A pseudopotential model for Dirac electrons in graphene with line defects

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Abstract
We consider electron transport in a planar fermion model containing various types of line defects modeled by $\delta$-function pseudopotentials with different matrix coefficients. After determining the necessary boundary conditions, the transmission probability for electron transport through the defect line is obtained for various types of pseudopotentials. For the schematic model considered, which may describe a graphene structure with different types of linear defects, the valley polarization is obtained.

Keywords: low-dimensional models, line defect, valley polarization, graphene

(Some figures may appear in colour only in the online journal)

1. Introduction
Recent years have seen a particular interest in $(2+1)$-dimensional models in condensed matter physics. An important prototype of such models is graphene [1–3], a planar monatomic layer of carbon atoms, which may be regarded as a superposition of two triangular sublattices, A and B, forming a hexagonal lattice. As has been recently discovered, graphene possesses various unusual properties. For instance, in [4, 5] properties such as the anomalous Hall effect, conductivity and other interesting features of the material were investigated. The behavior of electrons in problems related to graphene can be effectively described by the Dirac equation for massless fermions obtained from a continuum version of the tight-binding model [6–9]. A chiral gauge theory for graphene was formulated in [10]. Further studies of the theory of two-dimensional tight-binding quantum systems, as described in the continuum approximation by the Dirac equation in $(2+1)$-dimensional space–time with account for topological properties, were made in [11–13]. Note that, despite its similarity, this equation is not a relativistic wave equation in this context, but arises by linearizing the energy as a function of the momentum near the Dirac points, i.e. the intersections of the energy dispersion with the Fermi level.

Recently, models with different types of defects in the structure of planar systems have attracted a great deal of attention (see, e.g., [14–17]). These defects can lead to many nontrivial properties of the transmission of propagating particles, which are related to nonuniform densities near the defects and barriers. Recent investigations in graphene have provided various examples of this kind of problem. Let us mention, in particular, the experimentally observed topological line defect, containing the periodic repetition of one octagonal plus two pentagonal carbon rings along a certain direction embedded in a perfect graphene sheet [14], and also interesting grain boundaries [15] in graphene. Clearly, more new important applications of low-dimensional structures can be realized, once transport problems within them are well understood. In particular, as line defects have a simple geometry, this makes them easier for a theoretical study and suitable for use for controlled transport in graphene. In this context, let us mention recent theoretical studies of electronic transport through a line defect in graphene considered in [16], which were based upon the Green function approach.

The aim of this paper is to study line defects as barriers for electron propagation by using the effective Dirac equation for electrons in (monolayer) graphene [4–8] in the framework of a schematic pseudopotential model. Our motivation for considering such a model is based on the concept of effective, induced gauge fields which arise from perturbations in the hopping parameters of the tight-binding model [5, 9, 18] and were introduced in order to describe defects in graphene.
Thus, our starting point will be a general expression for the Hamiltonian, including effective, induced gauge potentials and a mass-type term. On this basis, we shall then consider all possible types of barrier-type perturbations in configurations of gauge fields and the mass-type term, chosen for convenience at the same position \( x \) and described in the limiting case by a pseudopotential term \( W(x) \) which depends on the pseudospin (sublattice) and valley (Dirac point) indices. In this way, the problem of describing line defects in planar systems can be mapped to a delta-function pseudopotential \( W(x) = W_0(x) \), where the matrix factor \( W \) contains the parameters characterizing the strength of interactions combined with Pauli matrices, mimicking the pseudospin and valley structure of the defect line. After determining the required boundary conditions, we can then find exact analytic solutions in a simple way. Comparison of our general results with some special cases of defects, such as the defect containing pentagonal and octagonal carbon rings \([14, 16]\), confirms our assumption that defects in graphene can be described by a Hamiltonian containing effective vector and scalar potentials, which are induced by changes in the nearest-neighbor (NN) or next-nearest-neighbor (NNN) hopping amplitudes.

The paper is organized as follows. In section 2 we introduce the general expression for the Hamiltonian containing induced gauge potentials and a mass-type term and give some motivations for how to arrive at the corresponding pseudopotential as a delta-function-limit of more realistic barrier-type field configurations. Section 3 contains the derivation of the necessary boundary conditions for the Dirac equation with a pseudopotential and provides explicit expressions for the transmission probability and the valley polarization describing electron transport through the defect line. A comparison with other models like the scalar potential barrier and the defect line containing pentagonal and octagonal carbon rings is also performed. Section 4 gives a discussion of numerical results and section 5 contains a summary and conclusions.

2. The pseudopotential for the effective 2D Dirac equation

Consider a planar system modeling monolayer graphene with electrons in \( D = 2 + 1 \) space–time. Different physical mechanisms give rise to (perturbative) interaction terms in the effective Dirac Hamiltonian that describes electrons in graphene. These perturbations may arise due to several types of disorder, like topological lattice defects, strains and curvature. Such defects are expected to exist in graphene, as experiments show a significant corrugation in suspended samples, in samples deposited on a substrate, and also in samples grown on metallic surfaces (see, e.g., \([18, 19]\), and references therein). Note, in particular, that changes in the distance between the atoms and in the overlap between the different orbitals by strain or bending lead to changes in the NN-hopping or NNN-hopping amplitude, and this results in the appearance of vector potentials \( A_1(\mathbf{r}) \), \( A_2(\mathbf{r}) \) (this coupling must take the form of a gauge field with the matrix structure of the Pauli matrices, \( \sigma_1 \) and \( \sigma_2 \)) and a scalar potential \( V(\mathbf{r}) \) in the Dirac Hamiltonian \([5, 9, 18]\). Moreover, in a region of finite mass the Hamiltonian for the Dirac electrons should include an \( \mathbf{r} \)-dependent mass term \( m(\mathbf{r}) \) (\( m(\mathbf{r}) \) is the effective mass with a \( \sigma_3 \) matrix), due to which the electronic spectrum will possess a finite energy gap. Practically, this type of term can be generated by covering the surface of graphene with gas molecules \([20]\), or by depositing graphene on top of boron nitride \([21, 22]\).

Let us therefore start with the following general expression for the Hamiltonian including the induced gauge potentials and a mass-like term:

\[
\mathcal{H} = \sum_{\mathbf{r} = \pm 1} \int d^2x \left[ \Psi^\dagger_\tau(\mathbf{r}) \left( \sigma_1 [-i \partial_x A_1(\mathbf{r}) - A_2(\mathbf{r}) - \mathbf{A}(\mathbf{r}) \cdot \mathbf{v}_F] \right) \Psi_\tau(\mathbf{r}) + \right. \\
+ \left. \tau \sigma_2 [-i \partial_y A_1(\mathbf{r})] \Psi_\tau(\mathbf{r}) \right] + \sum_{\mathbf{r} = \pm 1} \int d^2x \left[ \Psi^\dagger_\tau(\mathbf{r}) \left( \sigma_3 \mathbf{r} \right) \Psi_\tau(\mathbf{r}) + \right. \\
+ \left. V(\mathbf{r}) I \Psi_\tau(\mathbf{r}) \right].
\]

Here, the spinors in the 2D plane, \( \Psi_\tau(\mathbf{r}) \) (\( \tau = \pm 1, \mathbf{r} = (x, y) \)), have two components,

\[
\Psi_\tau(\mathbf{r}) = \begin{pmatrix} \psi_{1,\tau} \\ \psi_{2,\tau} \end{pmatrix},
\]

describing electrons at the two A, B sublattices \( (i = 1, 2) \); \( \sigma_1 \) are \( 2 \times 2 \) Pauli-matrices, \( I \) is the unit matrix and \( \psi_F \) is the Fermi velocity \(^4\).

The physical spin of the electrons that is due to the spatial rotation properties of the electron wavefunction has been neglected in our analysis, and the spinor nature of the wavefunction has its origin in the sublattice degrees of freedom, called pseudospin. The subscript \( \tau = \pm 1 \) stands for the two Fermi points \( K, K' \), corresponding to valleys at the corners in the first Brillouin zone, and plays the role of a flavor index. Besides the above effective gauge fields an effective electrostatic potential barrier may also influence the electron propagation in graphene (see, e.g., \([23]\)). The term that is responsible for this (and equally magnetic) interaction may be included in the Hamiltonian just as an electrostatic scalar potential \( e\Phi(\mathbf{r}) \) (and vector potential \( e\mathbf{A}_{\text{dir}}(\mathbf{r}) \)). The corresponding property of ‘relativistic’ Dirac electrons in graphene is their ability to tunnel through such a potential barrier with probability one. This is the so-called Klein tunneling of chiral particles (see, e.g., \([23]\))^5. Its presence in graphene is undesirable for graphene applications to nanoelectronics.

\(^3\) Note that the induced gauge field \( \mathbf{A} = (A_1, A_2) \) couples as a complex field \( \mathbf{A} = A_1 + iA_2 \) to the pseudospin spinor components, whereas the scalar potential \( V \) is real. At the other Fermi point one has to take the complex-conjugate field \( A^\ast \) \([5, 9]\). For simplicity, we discard here a (small) chemical potential-type term arising from the NNN-hopping energy.

\(^4\) Our choice of signs in front of the momentum and vector potential components of the Hamiltonian essentially corresponds to the conventions of \([4, 9]\). It may differ from that of other papers due to the adoption of different initial definitions. However, the final results do not depend on it. As usual, we use units such that \( \hbar = 1 \).

\(^5\) For the Klein paradox of relativistic electrons, see the original article \([24]\).
In order to overcome this difficulty, one may generate a gap in the spectrum, which is equivalent to the generation of a space-dependent mass term. Clearly, the simultaneous existence of a scalar potential barrier and a vector gauge field $A = (A_x, A_y)$ in some spatial regions may influence the electron transmission, say, in the $x$-direction. In order to study the possible joint role and competition of these perturbations, we combined them in the model Hamiltonian (1).

In this way, we assume that the motion of electrons is described by the planar Dirac equation $H_t \Psi_t = i\hbar \frac{\partial}{\partial t} \Psi_t$ with the Dirac Hamiltonian operator

$$H_t = \sigma_1 \left[ -v_F i \partial_x - A_x(\vec{r}) \right] + \sigma_2 \left[ -v_F i \partial_y - A_y(\vec{r}) \right] + i\hbar \tau \left[ \sigma_3 + V(\vec{r}) I \right]$$

where $\tau = \pm 1$ is the valley index. The expression (3) implies that the low-momentum expansion around the other Fermi point with $\tau \to -\tau$ gives rise to a time-reversed Hamiltonian. Note that the total effect of both valleys, as described in 4-spinor notation [8] (and references therein), respects time-reversal invariance. Let us now assume that the possible defects considered are lying in the same spatial region taken, for simplicity, to have the form of a line lying on the $y$-axis ($x = 0$). Therefore, our study is considered as the investigation of a delta-function limit of more realistic barrier-type configurations and may be based on the schematic model Hamiltonian

$$H_t = -i\sigma_1 \partial_x - i\tau \sigma_2 \partial_y + W_t(x),$$

where we have introduced the pseudopotential $W_t(x)$,

$$W_t(x) = V(x) I - A_x(x) \sigma_1 - \tau A_y(x) \sigma_2 + m(x) \sigma_3,$$

which in the delta-function limit can be written in the form

$$W_t(x) = W_t \delta(x) = (a I - b_1 \sigma_1 - b_2 \tau \sigma_2 + b_3 \sigma_3) \delta(x).$$

In equation (4), and in what follows, the Fermi velocity, with the corresponding choice of the units, is supposed to be equal to unity, $v_F = 1$. The scalar and vector potentials and the mass-type term are chosen as $V(x) = an(x)$, $A_x = b_1 \delta(x)$, $A_y = b_2 \delta(x)$, $m(x) = b_3 \delta(x)$, where $a$, $b_i$ ($i = 1, 2, 3$) are constants that describe the interactions of particles in sublattices on either side of the line defect and are related to the ‘hopping parameters’ (see below).

Let us now apply the above schematic model to graphene with line defects, arising in the form of deformations in the structure or displacements of carbon atoms in the hexagonal crystal lattice (some of these defects were, e.g., described in [25, 26]).

The $(2 + 1)$-dimensional Dirac equation for the model under consideration,

$$i\hbar \frac{\partial}{\partial t} + i\sigma_1 \partial_x - \tau \sigma_2 p_y - W_t \delta(x) \right] \Psi_t = 0,$$

has stationary solutions

$$\Psi_t(\vec{r}, t) = \left( \Psi_{1,t}, \Psi_{2,t} \right) e^{i p_x x} e^{-iEt},$$

where the functions $\Psi_{i,t}(x)$ ($i = 1, 2$) should be found by a limiting procedure [7] around the defect line $x = 0$. The solutions of the free Dirac equation for $\tau = +1$ (for $\tau = -1$ the corresponding solution is also easily found) in the $x < 0$ and $x > 0$ regions can be written respectively as (to simplify the notation, we omit here the subscript $\tau = +1$)

$$\begin{align*}
\Psi_1 &= \left( 1 \right) e^{i p_x x} e^{-iEt} + B \left( -e^{-iEt} \right) e^{-iE t}, \\
\Psi_2 &= C \left( 1 \right) e^{i p_x x} e^{-iEt},
\end{align*}$$

where $B$ is the incident angle of the electron wave with respect to the $x$-axis, $p_x = p \cos \beta$, $p_y = p \sin \beta$.

3. Transmission through the pseudopotential

Let us next study the transmission through the defect line in two particular cases of main interest: $(1) b_1 \neq 0$, $a = b_2 = b_3 = 0$, and $(2) b_1 = 0$, $a \neq 0$, $b_2 \neq 0$, $b_3 \neq 0$.

3.1. $b_1 \neq 0$, $a = b_2 = b_3 = 0$

The Dirac equations now take the form

$$E \Psi_1 + i \Psi_2 = i \tau p_y \Psi_2 + b_1 \delta(x) \Psi_2 = 0,$$

$$E \Psi_2 + i \Psi_1 = -i \tau p_y \Psi_1 + b_1 \delta(x) \Psi_1 = 0,$$

where $\Psi'_i = d\Psi_i/dx$.

By multiplying the first equation by $\Psi_1$, the second by $\Psi_2$ and, then, in order to exclude the $\delta$-function, subtracting the equations we obtain

$$E (\Psi_1^2 - \Psi_2^2) + i (\Psi_1 \Psi_2' - \Psi_2 \Psi_1') + 2i \tau p_y \Psi_1 \Psi_2 = 0.$$  

By dividing this equation by $\Psi_1^2$, integrating over $x$ between $-\epsilon$ and $+\epsilon$ ($\epsilon \to 0$) and assuming that the discontinuities of the functions are finite, we find the first boundary condition

$$\Psi_2 \bigg|_{x = +\epsilon} = 0,$$

$$\Psi_1 \bigg|_{x = -\epsilon} = 0.$$  

The problem of the solution of the low-dimensional Dirac equation with a delta-function potential was described in [27–29] (see also the discussion of the problem in [30–32]). There the authors have shown that the definition of $\Psi$ on the boundary of the barrier, which corresponds to an integration of the $\delta$-function with the prescription in the limit $\epsilon \to 0$ as follows: $\int_{-\epsilon}^{+\epsilon} \, dx \, \delta(x) f(x) = \frac{1}{2} \left[ f(+\epsilon) + f(-\epsilon) \right]$, is unphysical, if one considers the $\delta$-potential as a limit of the potential barrier. In what follows, it will become clear that the method used in the present paper can be considered as appropriate for the description of the limiting case of a narrow potential barrier, when the width of the short-range ' $\delta$-function' potential is considered larger than or comparable to the width of the interval where the function $f$ suffers a jump. Using this method, our result will be shown to be in full agreement with the result of the authors of [23] on the Klein paradox in the limit of a very high and narrow barrier.
Now, divide the first equation in (11) by $\Psi_2$, the second by $\Psi_1$, and integrate both equations over $x$ between $-\varepsilon$ and $+\varepsilon$ ($\varepsilon \to 0$). The new boundary conditions are

\[
\left. i \log(\Psi_2) \right|_{-\varepsilon}^{+\varepsilon} = -b_1, \\
\left. i \log(\Psi_1) \right|_{-\varepsilon}^{+\varepsilon} = -b_1.
\]

(14)

Upon substitution of the solution for the free Dirac equation (9) and (10) in (13) and (14), the transmission probability for both values of the valley indices, $\tau = \pm 1$, is found to be equal to unity,

\[
T_{\sigma_1} = |C|^2 = 1.
\]

(15)

This result can easily be explained from the point of view of the graphene structure. In the two-dimensional graphene model the spinor basis can be written in the form $\Psi_{\tau} = (\Psi_{1,\tau}, \Psi_{2,\tau})$, where $\Psi_{1,\tau}, \Psi_{2,\tau}$ are related to the A, B sublattices of graphene. The $\sigma_1$ matrix in front of the $\delta(x)$-function in the Dirac equation interchanges the A and B sublattice components in the wavefunction. However, in the tight-binding model of graphene one sums all terms over one sublattice, either A or B, and the corresponding nearest neighbors of the other sublattice, so that the graphene model is invariant under the transformation $A \rightarrow B, B \rightarrow A$. For this reason, the incident wave propagates without any reflection, since in this case the potential $-b_1 \delta(x) \sigma_1$ does not form any barrier for it.

3.2. $b_1 = 0, a \neq 0, b_2 \neq 0, b_3 \neq 0$

Consider the more general case with $a, b_2, b_3 \neq 0$, and only $b_1 = 0$. The Dirac equation (7) now takes the form

\[
[E + i\sigma_1 \partial_x - \tau \sigma_2 p_x - \delta(x) \\
\times (a I - b_2 \tau \sigma_2 + b_3 \sigma_1)]\Psi_{\tau} = 0,
\]

(16)

which transforms to the set of equations (omitting the index $\tau$ in the wavefunction)

\[
E \Psi_1 + i \Psi_1' + i r_2 \Psi_2 - \delta(x) (a \Psi_1 + i r_2 \Psi_2) = 0, \\
E \Psi_2 + i \Psi_2' - i r_2 \Psi_1 - \delta(x) (a \Psi_2 - i r_2 \Psi_1) = 0.
\]

(17)

After performing some further transformations and subsequent integration in the above equations to avoid problems with the delta-function (analogously to what was done in the previous section), we arrive at the expression

\[
\frac{1}{N} \arctan \left( \frac{1}{N} \left( (a + b_3) \frac{\psi_1}{\psi_2} + i r_2 b_2 \right) \right) \bigg|_{-\varepsilon}^{+\varepsilon} = i,
\]

(18)

where $N = \sqrt{b_2^2 + b_3^2 - a^2}$.

Substituting $\psi_1$, $\psi_2$ with the wavefunctions $\Psi_i(x = \pm \varepsilon)$ from equations (9) and (10), we find the transmission probability for both values of the valley index $\tau = \pm 1$,

\[
T_{I,\sigma_2,\sigma_1} (\tau) = |C|^2 = 1 - |B|^2
\]

\[
= \frac{\cos^2 \beta}{\cosh^2 N \cosh \beta + \frac{(a - b_2 \tau \sin \beta)^2}{b_2^2 + b_3^2 - a^2} \tanh^2 N},
\]

(19)

For a beam of electrons propagating towards the line defect, the scattered electrons will now be valley-polarized. The valley polarization, defined as [33]

\[
P_\tau = \frac{T_{(\tau = +1)} - T_{(\tau = -1)}}{T_{(\tau = +1)} + T_{(\tau = -1)}},
\]

(20)

thus takes the form

\[
P_\tau = \frac{2a b_2 \sin \beta \tanh^2 N}{\cos^2 \beta (b_2^2 + b_3^2 - a^2) + (a^2 + b_3^2 \sin^2 \beta) \tanh^2 N}.
\]

(21)

As can be seen from the above formula, the valley polarization becomes equal to zero for the incident angle $\beta = 0$.

3.3. Comparison with other models

It is instructive to compare the results of the previous section, where we have admitted three matrix coefficients in front of the $\delta(x)$-function, $I, \sigma_2, \sigma_3$, with some special cases considered in the literature.

3.3.1. Scalar potential barrier [23]. Clearly, the unit matrix $I$ in equations (1), (6) corresponds to diagonal pseudospin transitions $A \rightarrow A, B \rightarrow B$ with respect to the defect line, i.e. the graphene to the left of the defect line is mirror symmetric to the graphene on the right side of the defect line. This corresponds, e.g., to the model of graphene with a scalar (electrostatic) potential barrier of rectangular shape considered in [23],

\[
V(x) = \begin{cases} 
V_0, & 0 < x < D \\
0, & \text{otherwise}. 
\end{cases}
\]

(22)

The authors of [23] obtained the transmission probability for this model,

\[
T_D = \frac{\cos^2 \beta}{1 - \cos^2 (q_D) \sin^2 \beta},
\]

(23)

where $q_D = \sqrt{(E - V_0)^2/h^2 v_F^2 - k_F^2}$. Note that, in the limit $D \to 0$, $V_0 \to \infty$, $q_D D \to \infty$, where $D$ and $V_0$ are the potential barrier width and height, this result goes over to our expression (19) for the transmission probability for a delta-barrier, if we put $b_2 = b_3 = 0$, $a \neq 0$, with $q_D D = a$,

\[
T_a = \frac{\cos^2 \beta}{1 - \cos^2 a \sin^2 \beta}.
\]

(24)

3.3.2. Defect line containing pentagonal and octagonal carbon rings [14, 16]. Let us next consider the model of graphene with a defect line, containing pentagonal and octagonal carbon rings, described, e.g., in [14, 16, 25, 26]. In [16], with the use of the tight-binding lattice model and the Green function formalism the authors obtained the following result for the transmission probability in the low energy limit:

\[
T_{(\tau = \pm 1)} = \frac{\tau_1^4 \cos^2 \beta}{(\tau_1^4 + \tau_2^4) \pm 2 \tau_1 \tau_2 \sin \beta},
\]

(25)
where \(\tau_1, \tau_2\) are NN-‘hopping parameters’ (see figure 1). Using the notation of the authors, \(x = \tau_2/\tau_1^2\), one can rewrite (25) as follows:

\[
T_{(\tau=\pm1)} = \frac{\cos^2 \beta}{1 + x^2} \mp 2x \sin \beta.
\]  

To compare this expression with our results, let us consider equation (19) in the particular case when \(b_3 = 0\), i.e. when the effective mass-type term is neglected. There arises an interesting structural similarity with (26), if the parameters \(a, b_2\) of diagonal and non-diagonal pseudospin interactions in the pseudopotential (6) are not taken independently, but are assumed to satisfy the following relation:

\[
\frac{b_2^2}{a^2} = \cosh^2(N),
\]

where now \(N = \sqrt{b_2^2 - a^2}\). By inserting (27) into the expression (19) and putting \(b_3 = 0\), we obtain in the framework of our schematic model

\[
T_{I, \sigma_2} = \frac{\cos^2 \beta}{\cosh^2(N) [(1 + \frac{a^2}{b_2^2}) - 2 \tau \frac{a}{b_2} \sin \beta]} = \frac{\cos^2 \beta}{(1 + \frac{b_2^2}{a^2}) - 2 \tau \frac{b_2}{a} \sin \beta}.
\]

It should be noted that equation (27) has, besides the trivial solution \(\tau = 1\), a nontrivial solution for the ratio \(\frac{b_2}{a} \neq 1\), if \(a < 1\). This can be seen from figure 2. It is clear that for \(a \geq 1\) there exists only the trivial solution \(\frac{b_2}{a} = 1\), and the transmission probability can reach in this case its maximum value \(T_{I, \sigma_2} = 1\) for \(\beta = \pm \frac{\pi}{2}\) (\(\tau = \pm 1\)). It is amazing to note that our result (28) indeed looks similar to the expression (26), derived in [16] as a low energy limit in a much more involved calculation. By identifying the expressions \(b_2/a = \tau_2/\tau_1^2 = x\), it thus could be suggested that the coefficients \(a, b_2\) in our pseudopotential model effectively correspond to the hopping parameter quantities \(\tau_1^2\) and \(\tau_2\), respectively. In this way, one may conclude that \(a\) mimics the NNN diagonal pseudospin transitions of electrons via two neighboring pentagons of the linear defect in figure 1, giving \(\tau_1\)-hopping squared, whereas \(b_2\) is responsible for NN-hopping between two mismatched atoms of the B sublattice corresponding to \(\tau_2\). Obviously, such a correspondence between \(a, b_2\) and \(\tau_1^2\) and \(\tau_2\) supports the original interpretation of the role of these interactions in the pseudopotential (6) and looks like a concrete realization of the ideas of [5, 18], where the ‘scalar potential’ term \(a\delta(x)\) mimics the NNN-hopping, while the ‘vector-potential’ term \(b_2\sigma_2\delta(x)\) mimics the NN-hopping. Note that the above application and interpretation of the pseudopotential method required an important additional input, namely, the specific parameter relation equation (27), which apparently in some effective way reflects the internal microscopic structure of the defect line. Clearly, such an approach can offer only an approximate qualitative description of transmission phenomena.

4. Numerical results

Let us now return to the expressions for the transmission probability (19) and the valley polarization (21) of our schematic model for the case with \(a \neq 0\) and \(b_3 \neq 0\) simultaneously. The corresponding result could be useful for future research, because the transmission probability has a nontrivial behavior (see figure 3) and the valley polarization (21) equals zero only for zero incident angle, \(\beta = 0\).

The dependence of the transmission probability on the angle of incidence in the case \(b_2 = 0\), \(a \neq 0\), \(b_3 \neq 0\) is as follows:

\[
T_{I, \sigma_3} = (\cos^2 \beta)^2 \left( \cosh^2 \left( a \sqrt{\frac{b_2^2}{a^2} - 1} \right) \cos^2 \beta \right.
+ \sinh^2 \left( a \sqrt{\frac{b_2^2}{a^2} - 1} \right) \frac{1}{\left[ b_2^2/a^2 - 1 \right]^{1/2}} \right)^{-1}.
\]  

Figure 2. Solution of the equation \(\frac{b_2}{a} = \cosh N\) (see equation (27)) for different values of \(a\).
Its behavior is shown in figure 3. Obviously, if the contribution of the coefficient $b_3$ is greater than that of the coefficient $a$, the transmission is lower. However, if the contribution of the coefficient $b_3$ is lower than that of the coefficient $a$ for the same values of $a$, the transmission probability increases. As follows from equation (29), for values of $a \gg b_3$ it can reach the value $T = 1$ (for $\beta = 0$) (see figure 3).

As is known [19, 22], the term in the $D = (2 + 1)$ Hamiltonian (3) of the model with the $\sigma_3$ matrix corresponds to the effective mass of electrons, and as a consequence the electronic spectrum will present a finite energy gap. The existence of an energy gap prevents the Klein paradox\textsuperscript{8} from taking place, a necessary condition for the building of nanoelectronic devices made of graphene. Our conclusion supports the results of the authors of [19, 22] on the role of the mass term as a factor impeding the Klein tunneling of chiral electrons through the barrier. The valley polarization for the case $\beta = 0$ is still equal to zero. It should also be noted that our result (19), (29) for the transmission probability in the case with only $b_3 \neq 0$ corresponds to that of [22] in the limiting case of a narrow region with finite mass,

$$T_{\sigma_1}(\tau) = |C|^2 = 1 - |B|^2 = \frac{1}{\cosh^2 N}, \quad N = |b_3|. \quad (30)$$

Obviously, in the case $a = 0$ the valley polarization (21) equals zero at any angle, and the dependence of the transmission probability on the angle of incidence is described by the formula

$$T_{\sigma_1, \sigma_3} = (\cos^2 \beta) \left( \cosh^2 \left( b_2 \sqrt{b_3^2/b_2^2 + 1} \right) \cos^2 \beta \right. \right.$$  

$$+ \left. \sinh^2 \left( b_2 \sqrt{b_3^2/b_2^2 + 1} \right) \frac{\sin^2 \beta}{b_3^2/b_2^2 + 1} \right) \quad (31)$$

The interesting result in this case is that again the transmission is lower if the mass-type coefficient $b_3$ is greater than the coefficient $b_2$ (see figure 4 for various values of $b_2$).

\textsuperscript{8} The Klein paradox implies that impurities and the other most common sources of disorder will not scatter the electrons in graphene.

The third case corresponds to graphene with a defect line for $a \neq 0, b_2 \neq 0$ [16, 25, 26]. It follows from our general result (19) that

$$T_{I, \sigma_1} = (\cos^2 \beta) \left( \cosh^2 \left( a \sqrt{b_2^2/a^2 - 1} \right) \cos^2 \beta \right.$$  

$$+ \left. \sinh^2 \left( a \sqrt{b_2^2/a^2 - 1} \right) \times \left( 1 - \frac{(b_2/a) \tan \beta}{b_2^2/a^2 - 1} \right) \right)^{-1}. \quad (32)$$

The transmission is still higher for small values of $a$, and the maximum of transmission for the case $a \approx b_2$ is observed for the angles $\beta \rightarrow \pi/2 ((\tau = +1))$ and for the angles $\beta \rightarrow -\pi/2 (\tau = -1)$ (see figure 5(a)). If the contributions of the coefficients $a$ and $b_2$ are not equal ($a \gg b_2$ or $a \ll b_2$), the maximum of the transmission probability is shifted from the angles $\beta \approx \pm \pi/2$ towards the center of the graph. It should be noted that the transmission probability for the case $a \ll b_2$ is small, while for the case $a \gg b_2$ it tends to a maximum value of 1 (see figure 5(b)). The valley polarization for this case is given by (21), if we set $b_3 = 0$. The result for $a > 1$ is similar to that of [33] (see figure 6, black line). The polarization for $a \approx 1$ has an almost linear dependence on the angle $\beta$ (see figure 6, red line). However, for $a < 1$ the dependence of the valley polarization on the angle of incidence has a nontrivial behavior (see figure 6, blue line). The graphics of the valley polarization for different contributions of the coefficients $a, b_2$ are shown in figures 7(a) and (b).

5. Summary and conclusions

In this paper, we have studied a planar electron system for graphene containing a defect line with a pseudospin and valley structure by using a schematic model with a delta-function pseudopotential. The underlying structure of the considered pseudopotential is assumed to arise from various perturbations on the line, in particular strain, which lead to changes in the NN- and NNN-hopping amplitudes and are represented by vector and scalar gauge fields with the matrix structure of the...
The transmission probability $T$ for different valley indices $\tau = \pm 1$ as a function of the incident angle $\beta$ for $b_3 = 0$ and for different values of the parameter $a$ and ratio $b_2^2/a^2$.

The valley polarization $P$ as a function of the angle of incidence $\beta$ for $b_3 = 0$ and for different values of the parameter $a$ and ratio $b_2^2/a^2$.

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Sublattice (pseudospin) Pauli matrices and the unit matrix in the Dirac Hamiltonian. In addition, a space-dependent mass term, localized in a narrow region of space, was taken into account and described by including a delta-function term with $\sigma_3$ matrix coefficient. On this basis, the transmission through a defect line in the graphene structure with various types of pseudospin defects was considered, and the transmission probability and valley polarization were obtained in the framework of the considered schematic model. Moreover, we also presented justifications for dealing with the $\delta$-function pseudopotential as a model of a narrow square barrier by considering limiting cases of special interest. Note that in the limit of a narrow square barrier our calculation proved to be in agreement with the corresponding limit of the result of [23] obtained for an electrostatic potential barrier of finite width (Klein paradox). Moreover, the considered pseudopotential model also allows an interesting effective description of a defect line with linear repetition of two pentagonal and one octagonal carbon rings [14, 16]. In particular, it was shown that our results go over to those obtained earlier on the basis of the Green function method [16] if the parameters $a$, $b_2$ of diagonal and non-diagonal pseudospin interactions in the pseudopotential (6) are not taken independently, but are assumed to satisfy the specific relation (27).

We hope that the considered pseudopotential method and results of this paper will help to enlarge, at least qualitatively, our understanding of the transport problems of charged particles in planar configurations containing line defects with various pseudospin structures.

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Note added. After completion of this work, we became aware of the recent publications [34–36] studying defect lines in the continuum and tight-binding approach to graphene. These papers started from a constant potential for an extended defect line of width $W$ taken in the limit $W \to 0$. On this basis, they then delivered a detailed microscopic treatment of boundary conditions and the TB wave equations. In contrast, our (more phenomenological) approach starts from a low-energy continuum description of graphene which is based on a general expression for the Hamiltonian (compare equation (1)) containing deformation-induced gauge fields and a mass term which are subsequently modeled by a delta-function line singularity. Nevertheless, despite all conceptual and technical differences in the concrete calculations, their approach and ours lead to similar conclusions. It should also be mentioned that the results obtained in [34–36] after some transformations fully correspond to those of [16].

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