Abstract. We consider the energy spectrum of the planar quantum well which consisted of two ribbons of narrow-gap semiconductors and a graphene ribbon between ones. It is shown that the gapless mode appears only in case of inverted narrow-gap semiconductors. Spin splitting of the energy spectrum for a nonsymmetric quantum well is calculated taking into account a specificity of graphene. We investigate interface states and optical transitions. It is shown that the optical transitions are possible only with a conservation of a parity.

PACS numbers: 71.15.Rf, 73.21.Fg, 73.61.Wp, 73.63.Hs

Submitted to: Bulletin of the Lebedev Physics Institute

After the first experimental investigation of graphene, a monatomic layer of carbon atoms forming a regular hexagonal lattice [1, 2], an intensive activity has arisen in different directions. In particular, a multitude of works on electronic properties of narrow graphene ribbons with nanometer sizes (nanoribbons) of late three years were made. Among early ones, there were works on study of electron states of the graphene ribbons using the Dirac equation with the appropriate boundary conditions [3, 4]. The electronic properties of the graphene nanoribbon (GNR) depend strongly on size and geometry, as well as on whether hydrogen atoms were deposited on free atomic orbitals of carbon atoms at edges of the GNR [5]. In their transport properties, the GNRs are very similar to carbon nanotubes, since a free motion is one-dimensional (1D) in both cases [6, 7].

The boundary conditions for nanotubes, in which charge carriers are described by the Dirac equation, were discussed in detail in Ref. [8]. Two types of the boundary conditions correspond to two types of edges of the graphene ribbon, namely zigzag and armchair [3]. A formation of the zero-energy surface states is characteristic for the GNRs with the former type of edges. The energy spectrum is gapless (metallic) for the latter type of edges, when the ribbon width $d = (3M + 1)a$, where $M$ is an integer and $a = \sqrt{3}a_0$ is the lattice constant ($a_0$ is the interatomic distance), and insulating otherwise [4].

Recently, a transistor was made on the basis the GNR with the 2-nm width and 236-nm length (nanoribbons with the 10–60-nm width were also investigated) [9]. The GNR was taken so narrow to guarantee a wide semiconducting energy gap for room temperature operation of the transistor. However, it loses slightly a compactness to the transistor based on a graphene quantum dot with the 30-nm diameter [10].

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A planar contact of the GNR with zigzag edges with metal ribbons has been investigated in Ref. [11] within the tight-binding approximation. In our paper, we consider the size quantization of massless charge carriers in the GNR having armchair edges with the width $d \neq (3M + 1)a$ between narrow-gap semiconductor ribbons. Changing narrow-gap semiconductors, we can change potential barriers heights which are the band gaps of the narrow-gap semiconductors, what opens additional possibilities for the energy band-gap engineering [12].

The potential barrier height for the single GNR has been calculated in Ref. [13] within the local spin density approximation. It equals 2.33 and 3.33 eV for the armchair and zigzag edges, respectively. These values is one order higher than a typical band gap of the narrow-gap semiconductors.

We carried out calculations within the Dirac model [14]. Let us direct $X$ axis parallel to interfaces of the narrow-gap semiconductors and graphene, $Y$ axis transversely to a heterostructure plane, and $Z$ axis transversely to $X$ and $Y$ axes (Fig. 1). In a two-band approximation, a heterostructure composed of narrow-gap semiconductors and graphene is described by the Dirac equation. Half the band gap $\Delta$, the work function $V$, and the matrix element for the rate of interband transitions $u$ are constant and change only on the heterostructure boundaries. For chosen orientation of axes in given case, the Dirac equation has following form

$$\hat{H}_D \Psi \equiv \left\{ u_i \gamma^0 \gamma^1 \hat{p}_x + u_i \gamma^0 \gamma^3 \hat{p}_z + \gamma^0 \Delta_i + V_i \right\} \Psi = E \Psi, \tag{1}$$

where $\gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$ and $\gamma = \begin{pmatrix} 0 & \sigma \\ -\sigma & 0 \end{pmatrix}$ are the Dirac $\gamma$-matrices, $I$ is the $2 \times 2$ unit matrix, $\sigma$ are the Pauli matrices, $\hat{p} = -i \nabla$ is the momentum operator, and $\hbar = 1$.

It is simply verified that the operator

$$\hat{P} = i \gamma^0 \gamma^3 \gamma^1 \tag{2}$$

commutes with Hamiltonian $\hat{H}_D$.

To clear up the sense of the operator $\hat{P}$ we present it in the form

$$\hat{P} = i \gamma^0 \hat{\Lambda}_y, \tag{3}$$

where $i \gamma^0$ is the inversion operator, $\hat{\Lambda}_y = e^{-i \frac{\pi}{2} \Sigma_y} = -i \Sigma_y$ is the operator of the rotation about the $Y$ axis by angle $\pi$ (see, e.g., [17]), and $\Sigma_y = \begin{pmatrix} \sigma_y & 0 \\ 0 & \sigma_y \end{pmatrix}$. From this, one can see that the operator $\hat{P}$ plays the role of the pseudoparity operator introduced for the layered narrow-gap semiconductor heterostructures [18].

\[2\] We can use a finite-gap graphene modification as a narrow-gap semiconductor [15].

\[3\] One should distinguish the operator $\hat{P}$ from the helicity operator $\hat{h}$, introduced for unbounded graphene [16], which is the operator of a projection of pseudospin onto a free motion momentum. The free motion is 1D in the planar heterostructure and the 1D operator $\hat{h}$ (written in the $4 \times 4$ matrix form) does not commute with $\hat{H}_D$. Therefore, an eigenvalue of $\hat{h}$ does not conserve. The conserved quantum number is the eigenvalue of the operator $\hat{P}$. 

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The eigenvalues \( \lambda = \pm 1 \) of the operator \( \hat{P} \) determine sign of a spin projection onto \( Y \) axis. It can be verified by the calculation of the mean value of spin as it was made in Ref. [18]. Hereinafter, we will refer to \( \lambda \) as the parity. As it was emphasized in our previous paper [19], the charge carriers in graphene are the chirality massless Dirac fermions (spin of particle is aligned with its momentum or is opposed to it). As it will be shown below, there is no the gapless mode in the quantum well considered. The charge carriers in the GNR of a finite width bounded by layers of usual (noninverted) narrow-gap semiconductors, have nonzero effective mass and its energy spectrum is similar to the semiconductor spectrum with the finite band gap.

We find a solution to equation (1) in a class of functions being the eigenfunctions of the pseudoparity operator (2). Components of the eigen bispinor interconnect by relations

\[
\begin{align*}
\psi_{\lambda 2} &= i\lambda \psi_{\lambda 1}, \\
\psi_{\lambda 4} &= -i\lambda \psi_{\lambda 3}.
\end{align*}
\]

Now the Dirac equation (1) is written in the form

\[
\left\{ u_i \gamma^0 \gamma^3 \hat{p}_z - i\lambda \gamma^3 u_i k_x + \gamma^0 \Delta_i + V_i \right\} \Psi_{\lambda} = E_{\lambda} \Psi_{\lambda}.
\]
Two independent components of the eigen bispinor satisfy the system of equations

\[
\begin{align*}
\left(-iu \frac{d}{dz} + i\lambda u k_x\right) \psi_{\lambda 1} &= (E_\lambda + \Delta_i - V_i) \psi_{\lambda 3}, \\
\left(-iu \frac{d}{dz} - i\lambda u k_x\right) \psi_{\lambda 3} &= (E_\lambda - \Delta_i - V_i) \psi_{\lambda 1}.
\end{align*}
\]  

(6)

We find the solution in three ranges in the form

1) \( z < 0 \): \( \psi_{\lambda 1} = A_1 e^{k_1 z}, \psi_{\lambda 3} = A_3 e^{k_1 z}, \)
2) \( 0 < z < d \): \( \psi_{\lambda 1} = B_1 e^{ik z} + \tilde{B}_1 e^{-ik z}, \psi_{\lambda 3} = B_3 e^{ik z} + \tilde{\tilde{B}}_3 e^{-ik z}, \)
3) \( z > d \): \( \psi_{\lambda 1} = C_1 e^{-k_1 z}, \psi_{\lambda 3} = C_3 e^{-k_1 z}, \)

respectively, for the narrow-gap semiconductor with \( \Delta \) and the inverted narrow-gap semiconductors \[21\] in which \( \Delta \) correspond to

\( k \)

The gapless mode corresponds to

\( \psi \)

Using the boundary conditions of continuity of \( \sqrt{u} \Psi \) \[20\], one can exclude constants \( A_1, A_3, C_1, C_3, B_3, \tilde{B}_3 \) and obtain the system of equations on coefficients \( B_1 \) and \( \tilde{B}_1 \)\footnote{The system of equations in \( B_3 \) and \( \tilde{\tilde{B}}_3 \) is analogous to (7).}

\[
\begin{align*}
\left(\frac{u_2 k + i\lambda u_2 k_x}{E_\lambda} + \frac{iu_1 k_1 - i\lambda u_1 k_x}{E_\lambda + \Delta_1 - V_1}\right) B_1 + \left(\frac{-u_2 k + i\lambda u_2 k_x}{E_\lambda} + \frac{iu_1 k_1 - i\lambda u_1 k_x}{E_\lambda + \Delta_1 - V_1}\right) \tilde{B}_1 &= 0, \\
\left(\frac{u_3 k + i\lambda u_2 k_x}{E_\lambda} - \frac{iu_3 k_3 + i\lambda u_3 k_x}{E_\lambda + \Delta_3 - V_3}\right) B_1 e^{ik dz} + \left(\frac{-u_2 k + i\lambda u_2 k_x}{E_\lambda} - \frac{iu_3 k_3 + i\lambda u_3 k_x}{E_\lambda + \Delta_3 - V_3}\right) \tilde{B}_1 e^{-ik dz} &= 0.
\end{align*}
\]  

(7)

The dependence of energy on the allowed wave number \( k \) and the wave number of the free motion \( k_x \) is given by relation

\[
E_\lambda = \pm u_2 \sqrt{k^2 + k_x^2}.
\]  

(8)

The gapless mode corresponds to \( k = 0 \). Then the energy spectrum is linear one \( E_\lambda = \pm u_2 |k_x| \). However, from (7), one can see that then \( B_1 + \tilde{B}_1 = 0 \) and \( B_3 + \tilde{\tilde{B}}_3 = 0 \), what means that \( \Psi_\lambda \equiv 0 \), therefore this solution is not physical one.

The gapless mode in the quantum well based on graphene is possible if graphene is bounded by the inverted narrow-gap semiconductors \[21\] in which \( \Delta_1 \Delta_3 < 0 \), \( u_1 = u_2 = u_3 = u \) and \( V_1 = V_2 = V_3 = 0 \). The wave function is constant in the range \( 0 < z < d \) at \( k = 0 \), namely, \( \psi_{\lambda 1} = D_1, \psi_{\lambda 3} = D_3 \). After a substitution of this solution in (6), we obtain \( D_3 = \pm i D_1 \) and \( E_\lambda = \pm \lambda u |k_x| \). Joining solutions on boundaries \( z = 0 \) and \( z = d \), we find the wave function

1) \( \Psi^{(\pm)}_\lambda = C \Psi^{(\pm)}_\lambda e^{\pm \lambda k} \),
2) \( \Psi^{(\pm)}_\lambda = C \Psi^{(\pm)}_\lambda \),
3) \( \Psi^{(\pm)}_\lambda = C \Psi^{(\pm)}_\lambda e^{\pm \lambda (z-d)} \),

where

\[
\Psi^{(\pm)}_\lambda = \begin{pmatrix} 1 \\ i\lambda \\ \pm i \\ \pm\lambda \end{pmatrix}.
\]
A constant \( C \) is determined from the normalizing condition

\[
\int_{-\infty}^{\infty} dz \Psi_\lambda^* \Psi_\lambda = 1,
\]

\[
C = \frac{1}{2} \left[ \left( \frac{1}{|\Delta_1|} + \frac{1}{|\Delta_3|} \right) + d \right]^{-1/2}.
\]

The case \( D_3 = iD_1 \) corresponds to \( \Delta_1 < 0, \Delta_3 > 0 \), and \( E_\lambda = \lambda \omega k_x \). For \( D_3 = -iD_1 \), we obtain \( \Delta_1 > 0, \Delta_3 < 0 \), and \( E_\lambda = -\lambda \omega k_x \).

We consider below the case of the noninverted narrow-gap semiconductors with \( \Delta_{1,3} > 0 \) when there no the gapless mode. It is simply obtained the equation in \( k \) corresponded to the equation investigated in Refs. [22, 23]

\[
\tan kd = \frac{A(C + \tilde{C})}{1 + B(C - \tilde{C}) - C\tilde{C}},
\]

where

\[
A = \frac{u_2 k}{E_\lambda}, \quad B = \frac{\lambda u_2 k_x}{E_\lambda}, \quad C = \frac{u_1 k_1 - \lambda u_1 k_x}{E_\lambda + \Delta_1 - V_1}, \quad \tilde{C} = \frac{u_3 k_3 + \lambda u_3 k_x}{E_\lambda + \Delta_3 - V_3},
\]

\[
u_1^2 k_1^2 = \Delta_1^2 - (E_\lambda - V_1)^2 + u_2^2 k_x^2, \quad u_2^2 k^2 = (E_\lambda - V_2)^2 - \Delta_2^2 - u_3^2 k_x^2, \quad u_3^2 k_3^2 = \Delta_3^2 - (E_\lambda - V_3)^2 + u_3^2 k_x^2.
\]

In general case, equation (10) is sufficient awkward therefore we restrict oneself to a consideration of the particular cases for the defined types of the quantum wells.

**The symmetric quantum well.**

We refer to such quantum well in which \( V_1 = V_3 = V, \Delta_1 = \Delta_3 = \Delta, \Delta_2 = 0, V_2 = 0, u_1 = u_3 = \pi, u_2 = u \) as the symmetric quantum well. Equation (10) is reduced to the form

\[
\tan kd = \frac{u \pi k}{\sqrt{\Delta^2 - u^2 k_x^2}}.
\]

The dependence of energy on \( \lambda \) vanishes, therefore, there is no parity splitting. Equation (11) reduces to the most simple form at \( V = 0 \) and \( u = \pi \)

\[
\tan kd = \frac{\sqrt{\Delta^2 - u^2 k^2}}{uk}.
\]

From the last equation, one can simply find the number \( n_{e(h)} \) of branches in the electron (hole) size-quantization spectrum (in given case \( n_e = n_h = n \)). This number is to be to valid an inequality\(^5\)

\[
\pi(n - 1) \leq \frac{d\Delta}{u} < \pi n.
\]

It is evident from the graphical solution of equation (12) that the theorem of nonrelativistic quantum mechanics remains valid which states that there exists at least one level in an arbitrarily shallow 1D symmetric quantum well\(^6\).

\(^5\)It is interesting to note that there exists the solution to equation (12) in the case \( \frac{d\Delta}{u} = \pi n \). This corresponds to a level lying on boundary with the continuous spectrum.

\(^6\)In the nonsymmetric quantum well as in a nonrelativistic case (see, e.g., [24]), there can exist no one level.
The nonsymmetric quantum well of the first type.

So we refer to the quantum well with \( \Delta_1 = \Delta_3 = \Delta, \Delta_2 = 0, V_1 = -V_3 = V, V_2 = 0, u_1 = u_3 = \pi, u_2 = u \). Then, \( \lambda \) explicitly enters into equation (10) as \( \lambda k_x \). Hence, parity splitting (spin splitting) arises. Energy extrema are not at \( k_x = 0 \) and lie at \( k_x = \lambda k_x^* \). Hence, an energy depends on \( k_x - \lambda k_x^* \). We suppose that \( |V| \ll \Delta \). In the lowest order of \( V \), the dependence of energy on a momentum \( k_x \) is given by expression (8)

\[
E^{(0)}_\chi = \pm u \sqrt{k^{(0)2} + k_x^2},
\]

where \( k^{(0)} \) is the root of equation (11) at \( V = 0 \)

\[
\tan k^{(0)} d = \frac{k^{(0)} \sqrt{\Delta^2 - u^2 k^{(0)2} + (\pi^2 - u^2)k_x^2}}{u k^{(0)2} + (u - \pi)k_x^2}.
\]

In the next order of \( V \), we have\(^7\)

\[
E^{(1)}_\chi = \pm u \sqrt{k^{(0)2} + (k_x - \lambda k_x^*)^2}.
\]

With the same accuracy, the extremum energy \( \pm u k^{(0)} \) at \( k_x = \lambda k_x^* \) coincides with the extremum energy at \( k_x = 0 \) in the symmetric quantum well, and a difference between ones \( \delta E \) is a higher-order infinitesimal, namely, \( |\delta E| \ll u |k_x^*| \ll \Delta \). Expanding (15) to the second-order infinitesimal and remaining terms with \( k_x^*2 \) and \( k_x^* V \) as terms of the same infinitesimal, we obtain

\[
k_x^* = \frac{V}{\pi} \cdot \frac{\Delta}{F} \cdot \left[ 1 + \sqrt{1 + \frac{u k_0}{\Delta^2 - u^2 k_0^2} F} \right],
\]

where \( F = 2 \sqrt{\Delta^2 - u^2 k_0^2} + \frac{u k_0^2}{\sqrt{\Delta^2 - u^2 k_0^2}} \).

The nonsymmetric quantum well of the second type.

So we refer to the quantum well with \( \Delta_1 \neq \Delta_3, V_1 = V_3 = V, V_2 = 0, \Delta_2 = 0, u_1 = u_3 = \pi, u_2 = u \). We will suppose that a deviation from the symmetric quantum well is small \( \Delta_1 - \Delta_3 = 2\Delta', |\Delta'| \ll \Delta_{1,3} \). It is convenient to introduce the half-sum of the energy gaps \( \bar{\Delta} = \frac{\Delta_1 + \Delta_3}{2} \), and the energy gaps are expressed in terms of \( \bar{\Delta} \) and \( \Delta' \), \( \Delta_1 = \bar{\Delta} + \Delta', \Delta_3 = \bar{\Delta} - \Delta' \).

Analogously to the first type of the quantum well, we find the approximate solution in the form

\[
\tilde{E}^{(1)}_\chi = \pm u \sqrt{\tilde{k}^{(0)2} + (k_x - \lambda k_x^*)^2},
\]

where \( \tilde{k}^{(0)} \) is the root of equation for the symmetric quantum well (11), in which \( \bar{\Delta} \) is taken instead of \( \Delta \). Further, by analogy with previous case, one can obtain the formula

\[
k_x^* = -\frac{\Delta'}{\pi} \cdot \frac{b + \sqrt{b^2 + ac}}{a},
\]

\(^7\)The quadratic dependence of an energy on a momentum, which is valid at large values of \( \Delta_2 \), was used in Ref. [22].
where \( a = 2(\tilde{\Delta} + u\tilde{k}_0 - V)\sqrt{\Delta^2 - (u\tilde{k}_0 - V)^2} + \tilde{u}\tilde{k}_0(u\tilde{k}_0 - V)\sqrt{\Delta + u\tilde{k}_0 - V})/(\tilde{\Delta} + u\tilde{k}_0 - V), \ b = ((\tilde{u} - u)\tilde{k}_0 + V)(\tilde{\Delta} + u\tilde{k}_0 - V), \ c = \tilde{u}\tilde{k}_0(u\tilde{k}_0 - V)/((\tilde{\Delta} - u\tilde{k}_0 - V)\sqrt{\Delta^2 - (u\tilde{k}_0 - V)^2}); \ tilde{k}_0 \ is \ the \ root \ of \ equation \ (11) \ at \ k_x = 0 \ (we \ neglect \ the \ dependence \ of \ \tilde{k}^{(0)} \ on \ k_x). \)

The interface states.  

The interface states (IS) were first predicted by I. E. Tamm in 1932 [25]. This states are localized near the narrow-gap semiconductor–graphene interfaces\(^8\). The solution in the ranges \( z < 0 \) and \( z > d \) is found in the same form as for the size-quantization states and in the quantum well in the form

\[
\psi_{\lambda 1} = B_1 e^{-qz} + \tilde{B}_1 e^{qz}, \ \psi_{\lambda 3} = B_3 e^{-qz} + \tilde{B}_3 e^{qz}.
\]

The quantity \( q \) is connected with \( E_\lambda \) by the relation

\[
E_\lambda^2 = u_2^2 k_x^2 - u_2^2 q^2,
\]

therefore, the condition of an IS existence is the inequality\(^9\)

\[
|q| \leq |k_x|.
\]

The equation in \( q \) is analogous to (10) with only difference that there is \( \tanh qd \) instead of \( \tan kd \) and \( q \) enters into \( A \) instead of \( k \).

In order to valid inequality (21) for all values of \( k_x \), it is necessary that the solution \( q \) to this equation vanishes at \( k_x \to 0 \). Otherwise, the IS arise at some critical \( k_x \) or they are not exist. It is simply shown that there is no such point \( k_{x0} \neq 0 \) that \( |q(k_{x0})| = |k_{x0}| \) in the case \( q(k_x) \neq const \). The function graph \( |q(k_x)| \) at \( k_x \neq 0 \) lies either lower the straight line \( q = |k_x| \) (there exist the IS) or higher the line \( q = |k_x| \) (there exist no the IS). The analysis of the solution of the equation at small \( k_x \) is presented in Table 1.

In particular, the existence of the IS of one parity is possible. A consequence of this fact is a spin current along the interface. The mentioned effect can be used in spintronics [27].

The IS can exist for charge carriers of one sign. The IS are energetically more favorable than the size-quantization states. This fact results in accumulation of the IS by the charge carriers of one type. Thus at an optical excitation, a charge of one sign will be localized along the interface against the background of the uniformly distributed charge of opposite sign.

Recently, it was shown within the electrostatic approach that the charge is induced at boundaries of the single GNR on the substrate at applying of an electric field transversely to its plane [28]. We think that a similar effect is also possible in the considered heterostructure due to a predominant occupancy of the IS.

\(^8\)We note that analogous states arise in a single heterojunction with an intersection of the dispersion curves [23, 26]. They are not a specificity of the quantum well and can also arise in the quantum barriers [7].

\(^9\)Such inequality were considered in Ref. [11] where term “evanescent modes” is used instead of the term “IS”.
Table 1. The results of the analysis of the solutions of the equation for the IS with $|q| \leq |k_x|$.

|                | There are no the IS | There are the IS of only one parity | There are the IS of both parities |
|----------------|---------------------|-------------------------------------|----------------------------------|
| **Electrons**  | $\{ p_1 > 1 \}$    | $\{ p_1 \geq 1 \}$, $p_3 \leq 1$ | $\{ p_1 \leq 1 \}$, $p_3 \geq 1$ |
|                | $\{ p_3 > 1 \}$    | $p_1 \neq p_3$                      |                                  |
| **Holes**      | $\{ p_1 < 1 \}$    | $\{ p_1 \leq 1 \}$, $p_3 \geq 1$ | $\{ p_1 \geq 1 \}$, $p_3 \leq 1$ |
|                | $\{ p_3 < 1 \}$    | $p_1 \neq p_3$                      |                                  |

Notations $p_1 = \sqrt{\frac{\Delta_1 + V_1}{\Delta_1 - V_1}}$, $p_3 = \sqrt{\frac{\Delta_3 + V_3}{\Delta_3 - V_3}}$ are introduced. The particular case $p_1 = p_3 = 1$ corresponds to a lack of the IS at small $k_x$ for both electrons and holes (see the text).

The case $p_1 = p_3 = 1$ ($\Delta_1 = \Delta_3$ and $V_1 = V_3 = 0$) corresponds to the lack of the IS at small $k_x$ for both electrons and holes. The IS of both parities can exist at $|k_x| > k_{xc}$. In the case $u_1 = u_2 = u_3 = u$, it is simply obtained from (12)

$$\tanh qd = -\frac{\sqrt{\Delta^2 + u^2q^2}}{uq},$$

(22)

the right-hand part of (22) is negative and equation (22) has not solutions. Therefore in the case $p_1 = p_3 = 1$, an existence of the IS is possible only at $u \neq \pi$ and $|k_x| > k_{xc}$.

Now, let us analyse a formation of the IS at a change of the width $d$ of the quantum well. They can disappear at some critical width $d_c$ so that there are no the IS at $d \leq d_c$.

Let us determine a criterion of the existence of the IS at the defined width $d$. The equation in $q$ has the form

$$\tanh x = f(x),$$

(23)

where $x = qd$ and $f(x)$ tends to an asymptotic $f(x) \simeq x$ at large $x$. For the existence of the solution to equation (23), the following two-sided inequality must be valid

$$0 < f'(0) < 1.$$ 

(24)

In the general case of the nonsymmetric quantum well, inequality (24) can not be solved analytically and we present the results for the symmetric quantum well.

Let us consider the case of the symmetric quantum well with $V = 0$. This corresponds to $p_1 = p_3 = 1$. The IS arise only at $u > \pi$, otherwise $f'(0) < 0$. One can see that the qualitative criterion of the IS existence, the intersection of the dispersion curves for the conduction and valence bands of the narrow-gap semiconductor with the dispersion straight lines for graphene
The result obtained for $\Delta_1$ is realized. It should be expected that the IS exist for both electrons and holes. As it was noted above, the IS arise at momenta of the free motion higher some critical momentum

$$|k_x| > k_{xc} = \frac{1}{\sqrt{2d}} \sqrt{\frac{u + \bar{u}}{u - \bar{u}}} \left\{ \sqrt{1 + \frac{4d^2 \Delta^2}{(u + \bar{u})^2}} - 1 \right\}^{1/2}. \quad (25)$$

The IS exist if the inequality $|q(k_{xc})| < |k_x|$ is valid. It provides along with the condition of the lack of the intersection $|q(k_x)|$ with the straight line $q = |k_x|$ a fulfillment of inequality (21) in the whole range $|k_x| > k_{xc}$.

The fact, that the IS begin at some critical momentum of the free motion, is in accord with the result obtained for $\Delta_1 = \Delta_2 = \Delta_3$ and $V_1 = V_2 = V_3$ in Ref. [29].

For $V \neq 0$ and $u = \pi$, the IS arise at $E_\lambda V < 0$. They exist for electrons when $V < 0$, i.e. $p_1 = p_3 < 1$, and for holes when $V > 0$, i.e. $p_1 = p_3 > 1$. There are the intersections of the straight lines of graphene with the dispersion curves either for the conduction band (there is the IS for electrons) or for the valence band of the narrow-gap semiconductor (there is the IS for holes). The critical momentum is

$$k_{xc} = \frac{1}{d^2|V|} \left( -u + \sqrt{u^2 + (\Delta^2 - V^2)d^2} \right). \quad (26)$$

**The optical transitions.**

In presence an electromagnetic wave $A = eAe^{i(qr - \omega t)}$ where $e$ is the polarization vector of the electromagnetic wave, the Dirac equation takes the form

$$\left\{ u_i \gamma^0 \gamma \left( \hat{p} - \frac{e}{c} A \right) + \gamma^0 \Delta_i + V_i \right\} \Psi = i \frac{\partial}{\partial t} \Psi. \quad (27)$$

The operator $\hat{O} = -\frac{\epsilon}{c} u_i \gamma^0 \gamma A$ is considered as a perturbation. The matrix element of this operator is expressed by the matrix element of the rate $v = e \cdot v$ for the interband transition from the valence to conduction band $E_\lambda \to E'_\lambda$ [18]

$$v = u_i \langle \Psi_\lambda | \gamma^0 \gamma | \Psi_\lambda \rangle, \quad (28)$$

where $u_i$ implies that $u_1$, $u_2$ and $u_3$ are used for $z < 0$, for $0 < z < d$, and $u_3$ for $z > d$, respectively, at calculation (28).

The calculation of the matrix element of the rate by formula (28) for the size-quantization gives

$$v_x = 2\lambda \delta_{\lambda \lambda'} A_1^* A_1 \left\{ i(a^* - a) \frac{u_1}{2k_1} + iu_2 \left[ (b^*_+ b - b_+ b^*) + f^* f(b^*_+ b - b_+ b^*) \right] d + (f^* b^*_+ b +$$

$$+ f^* b^*_+ b) \frac{e^{2ikd} - 1}{2ik} - (f b^*_+ b + f b^*_+ b) \frac{1 - e^{-2ikd}}{2ik} \right\} + i(c^* c - c^* c) \frac{u_3}{2k_3} e^{-2kd}, \quad (29)$$

$$v_z = 2\delta_{\lambda \lambda'} A_1^* A_1 \left\{ (a + a^*) \frac{u_1}{2k_1} + u_2 \left[ (b^*_+ b + b^*_+ b - f^* f(b^*_+ b + b_+ b^*) \right] d + (f^* b^*_+ b -$$

...}

9
Here, normalizing (9) results in the expression

$$-f^*b_+b_+\frac{e^{2ikd} - 1}{2ik} + (f^*b_- - f^*b_+b_+)\frac{1 - e^{-2ikd}}{2k} + (c^*c + \tilde{c}^*c)\frac{u_3}{2k_3}e^{-2kd} \right\}. \quad (30)$$

The coefficient $A_1$ is determined by normalizing condition (9)

$$2A_1^*A_1 = \left(1 + \frac{a^*a}{2k_1} + b^*b(1 + f^*f)(1 + \tilde{b}^*\tilde{b})d + \frac{b^*b}{2k} (f^* (\tilde{b}^2 - 1) + f((\tilde{b}^*)^2 - 1)) \sin (2kd) + \right.$$

$$\left. + \frac{i}{2k} \left( f^* (\tilde{b}^*)^2 - 1 - f((\tilde{b}^*)^2 - 1) \right) \sin^2 (kd) + \frac{c^*c + \tilde{c}^*c}{2k_3}e^{-2kd} \right)^{-1},$$

where

$$a = -i u_1 k_1 + i\lambda u_1 k_x, \quad b_+ = \tilde{b}b, \quad b_- = \tilde{b}^*b, \quad b = \frac{u_1}{u_2} \frac{1}{1 - f}, \quad \tilde{b} = \frac{u_2 k + i\lambda u_2 k_x}{E_\lambda},$$

$$\tilde{c} = \sqrt{\frac{u_1}{u_3}} e^{ikd} - f e^{-ikd} e^{kd}, \quad c = \frac{iu_3 k_3 + i\lambda u_3 k_x}{E_\lambda + \Delta_3 - V_3},$$

$$f = 1 + \frac{2u_2 k(E_\lambda + \Delta_1 - V_1)}{(-u_2 k + i\lambda u_2 k_x)(E_\lambda + \Delta_1 - V_1) + E_\lambda (iu_1 k_1 - i\lambda u_1 k_x)}.$$

For the calculation of the IS matrix element of the rate by formula (28), one should replace $k$ with $iq$

$$v_x = 2\lambda\delta_{\lambda\eta} A_1^* A_1 \left\{ i(a^* - a) \frac{u_1}{2k_1} + iu_2 \left[ -bb_+ \frac{1 - e^{-2gd}}{q} + 2fb(b_+ - b_-)d + f^2bb_- \frac{e^{2gd} - 1}{q} \right] + \right.$$  

$$\left. + iu_3 \tilde{c}(c^* - c) \frac{1 - e^{-2kd}}{2k_3} \right\}, \quad (31)$$

$$v_x' \equiv 0. \quad (32)$$

Here, normalizing (9) results in the expression

$$2A_1^*A_1 = \left(1 + \frac{a^*a}{2k_1} + 2f(b_+^*b_- - b^2)d + (b^2 + b_+^*b_+) \frac{1 - e^{-2gd}}{2q} + f^2(b^2 + b_+^*b_-) \frac{e^{2gd} - 1}{2q} + \right.$$  

$$\left. + (\tilde{c}^* + c^*c) \frac{e^{-2kd}}{2k_3} \right)^{-1}.$$  

It is evident from formulae (29)-(31) that only the transitions with the conservation of the parity is allowed (Fig. 2 shows them by arrows). The optical transitions for the IS exist only in the particular case $p_1 = p_3 = 1$ at an absorption of the electromagnetic waves with the linear polarization along the interfaces.

These conclusions can be experimentally verified by the following way. Let us take the symmetric quantum well. Applying a voltage $U$ to the GNR, one can achieve that the work function $V$ becomes equal to zero, i.e. the particular case $p_1 = p_4 = 1$ is realized at $U \neq 0$. Then the optical transitions arise. They are due to the absorption of the electromagnetic waves with an energy $E$ so that $E_{\text{min}} < E < \Delta_{\text{eff}}$ where $\Delta_{\text{eff}}$ is the effective energy gap in the size-quantization spectrum (the smallest energy difference between the electron and hole branches).
The possibility of the exciton formation.

In conclusion, we note that a formation of the finite effective energy gap in the size-quantization spectrum can result in the exciton generation at the optical pumping (the energy gap in graphene is zero and there are no excitons).

The ortoexcitons with the total spin \( S = 1 \) of an electron and a hole are direct in the the symmetric quantum well therefore they are short-lived, and the paraexcitons with \( S = 0 \) [30] are long-lived, since the transitions with the change in the parity are forbidden (out of the dependence wether they are direct or not). The ortoexcitons are indirect in the nonsymmetric quantum well (Fig. 2), therefore they must also be long-lived. It was noted earlier that the paraexcitons are short-lived for the layered narrow-gap semiconductor heterostructures because the transitions with the change of the parity are allowed [31].

The calculation of exciton binding energy in the planar quantum well based on graphene and the narrow-gap semiconductors represents a separate problem and it will be present elsewhere.

Fig. 2. Splitting of the energy spectrum in the nonsymmetric quantum well. The allowed transitions with the conservation of the parity are shown.
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