Original Research Articles

Energy Spectra of the Graphene-based Fibonacci Superlattice modulated by the Fermi Velocity Barriers

ABSTRACTS

The one-dimensional superlattice (SL) based on a monolayer graphene modulated by the Fermi velocity barriers is considered. We assume that the rectangular barriers are arranged periodically along the SL chain. The energy spectra of the Weyl-Dirac quasi-electrons for this SL are calculated with the help of the transfer matrix method in the continuum model. The Fibonacci quasi-periodic modulation in graphene superlattices with the velocity barriers can be effectively realized by virtue of a difference in the velocity barrier values (no additional factor is needed). And this fact is true for a case of normal incidence of quasi-electrons on a lattice. In contrast to the case of other types of the graphene SL spectra studied reveal the periodic character over all the energy scale and the transmission coefficient doesn't tend asymptotically to unity at rather large energies. The dependence of spectra on the Fermi velocity magnitude, on the external electrostatic potential as well as on the SL geometrical parameters (width of barriers and quantum wells) is analyzed. Results obtained can be used for applications in the graphene-based electronics.

Keywords: graphene, Fibonacci superlattice, velocity barriers.

1. INTRODUCTION

Graphene and the graphene-based structures draw the great attention of researchers in recent years. It is explained by the unique physical properties of graphene, and also by good prospects of its use in the nanoelectronics (see e.g. [1-4]). It is convenient to operate the behaviour of the Weyl-Dirac fermions in graphene by means of the external electric and magnetic fields, and a lot of publications are devoted to the corresponding problem for this reason. Recently one more way of controlling the electronic properties of the graphene structures, namely by means of the spatial change of the Fermi velocity was offered [5-10]. Some ways of fabrication of structures in which the Fermi velocity of quasi-particles is spatially dependent value were approved [5, 6]. This achievement of technology opens new opportunities for receiving of the nanoelectronic devices with the desirable transport properties.

It is known that the solution of this problem can be promoted in no small measure by use of the superlattices. This explains the emergence of a lot of publications in which the charge carriers behaviour in graphene superlattices of various types is investigated; these SL include the strictly periodic, the disordered ones, SL with barriers of various nature - electrostatic, magnetic, barriers of Fermi velocity. (As the last, we understand the areas of graphene where quasi-particles have different Fermi velocity, smaller or bigger than in the pristine graphene). Among the specified works, there are some devoted to the quasi-periodic graphene SL [11-15]. The quasi-periodic structures, as known, possess the unusual electronic properties of special interest (see e.g. [16]).

Motivated by the circumstances stated above we formulate the purpose of this work as follows: to study the main features of the energy spectra of the quasi-periodical graphene-based Fibonacci superlattices with the velocity barriers. We choose the Fibonacci SL because they are considered as the classical quasi-periodic objects, and the majority of the works associated with research of the quasi-periodic systems deals merely with them.

2. MODEL AND FORMULAE

Consider the one-dimensional graphene superlattice in which regions with various values of the Fermi velocity are located along the 0x axis: elements a and b refer to $\boldsymbol{v_a}$ and $\boldsymbol{v_b}$ velocities respectively. Elements a and b are arranged along SL according to the Fibonacci rule so that, for example, we have for the fourth Fibonacci generation (sequence): $s_4=abaab$. Generally, between the barriers corresponding to elements a and b, there is a quantum well for which the Fermi velocity is equal to unity as in a pristine graphene: $\boldsymbol{v_w}=\boldsymbol{v_0}$.

As we consider graphene in which the Fermi velocity is dependent on the spatial coordinate $\vec{r}$ i.e. $\vec{v}=\vec{v}(\vec{r})$ the quasi-particles submit to the massless Weyl-Dirac type equation:

$$-i\hbar\vec{\sigma}\cdot\nabla\left[\sqrt{\vec{v}(\vec{r})}\varphi(\vec{r})\right]\sqrt{\vec{v}(\vec{r})}=E\varphi(\vec{r}), \tag{1}$$

where $\vec{\sigma} = (\sigma_x, \sigma_y)$ the Pauli two-dimensional matrix, $\varphi(\vec{r}) = [\varphi_A(\vec{r}), \varphi_B(\vec{r})]^T$ two-component spinor, T transposing symbol. Introducing an auxiliary spinor $\Phi(\vec{r}) = \sqrt{\vec{v}(\vec{r})}\varphi(\vec{r})$ one can rewrite equation (1) as follows:

$$-i\hbar\vec{v}(\vec{r})\vec{\sigma} \cdot \nabla\Phi(\vec{r}) = E\Phi(\vec{r}). \tag{2}$$

Assume that the external potential consists of the periodically repeating rectangular velocity barriers along the axis 0x and potential is constant in each j-th barrier. The external electrostatic potential U may also be present and inside each barrier $U_j(x)$ = const (piece-wise constant potential). In this case, using the translational invariance of the solution over the 0y axis, it is possible to receive from the equation (2):

$$\frac{d^2\Phi_{\mathrm{A,B}}}{dx^2} + \left(k_j^2 - k_y^2\right)\Phi_{\mathrm{A,B}} = 0, \tag{3}$$

where indices A, B relate to the graphene sublattices A and B respectively, $k_j = \frac{[E-U_j(x)]}{v_j}$, measurement units $\hbar$=v_0=1 are accepted. If we represent the solution for eigenfunctions in the form of the plane waves moving in the direct and opposite direction along an axis Ox, we derive

$$\Phi(\mathrm{x}) = \left[a_j e^{iq_j x}\begin{pmatrix}1\\ g_j^+\end{pmatrix} + b_j e^{-iq_j x}\begin{pmatrix}1\\ g_j^-\end{pmatrix}\right], \tag{4}$$

where $q_j = \sqrt{k_j^2 - k_y^2}$ for $k_j^2 > k_y^2$ and $q_j = i\sqrt{k_y^2 - k_j^2}$ otherwise, $g_j^\pm = (\pm q_j + ik_y)v_j/E$, the top line in (4) pertains to the sublattice A, the lower one – to the sublattice B.
The transfer matrix, which associates wave functions in points x and $x+\Delta x$ reads

$$M_j = \frac{1}{\cos\theta_j}\begin{pmatrix}\cos(q_j\Delta x - \theta_j) & i\sin(q_j\Delta x)\\ i\sin(q_j\Delta x) & \cos(q_j\Delta x + \theta_j)\end{pmatrix}, \tag{5}$$

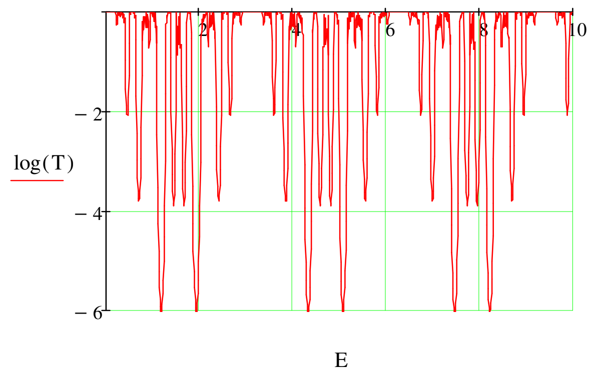
where $\theta_j = \arcsin\left(\frac{k_y}{k_j}\right)$.
Meaning that the Fermi velocity depends only on coordinate x, i.e. $v(\vec{r}) = v(x)$, it is possible to receive the boundary matching condition from the continuity equation for the current density as follows:

$$\sqrt{v_b}\varphi(x_{bw}^-) = \sqrt{v_w}\varphi(x_{bw}^+), \tag{6}$$

where indexes b and w relate to a barrier and a quantum well respectively, x_{bw} the coordinate of the barrier-well interface. The coefficient of transmission of quasi-electrons through the superlattice $\mathrm{T}(E)$ is evaluated by means of a transfer matrix method. Energy ranges, for which the coefficient of electron transmission through the lattice is close to unity, form the allowed bands, while the energy gaps correspond to values $\mathrm{T} \ll 1$. Since the specified procedure of obtaining the value of $\mathrm{T}(E)$ was described in literature repeatedly (see e.g. [7-14]) we have opportunity to proceed with analyzing the results obtained.

3. RESULTS AND DISCUSSION

Unlike the energy spectra for the known quasi-periodic superlattices, including the graphene ones (see e.g. [7, 14, 15]), the spectra of the graphene-based SL with the velocity barriers are periodic over all the energy scale, and the transmission rate T doesn't tend asymptotically to unity at rather large energies. For comparison, dependences of log $\mathrm{T}(E)$ are given in Fig. 1(a) for the Fibonacci fourth generation for SL in which the quasi-periodic modulation is achieved due to different values of the Fermi velocity, and for SL on the basis of the gapped graphene in which the quasi-periodic modulation is due to different values of gaps (calculations are carried out on the basis of our previous work [14], (Fig. 1(b)). The values of the parameters are as follows: for the first case w=1, d=2, v_a=1, v_b=2, for the second case w=d=1, Δ_a=1, Δ_b=0, where Δ denotes the gap's width, d and w denotes the barrier and the quantum well width respectively. All calculations (for all figures of this paper) were carried out for the case of the normal incidence of electrons on the superlattice. (Note that in accordance with the known Landauer-Buttiker formula the electrons with k_y = 0 make the main contribution to the conductance).



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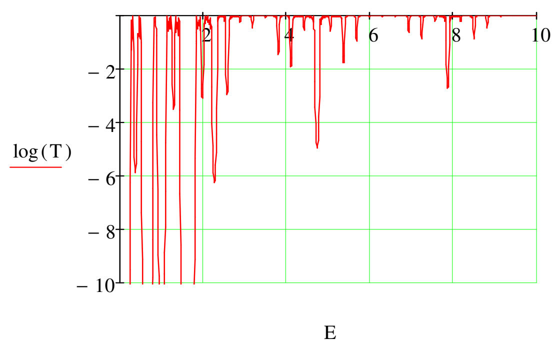


(b)

Fig. 1. Dependence of log(T) on energy *E* for the SL modulated by: (a) different values of the Fermi velocity and (b) different magnitudes of the energy gaps

It is seen that a certain periodicity of spectra takes place in the second case (this fact hasn't been noted in the literature as yet) but the amplitude of peaks (and the corresponding gap's width) decreases with increasing in E, on average. The allowed band width increases on average with E increasing and the coefficient of transmission T eventually approaches to unity. This "wavy damped oscillation" in Fig. 1(b) is associated with such property of the spectra as their self-similarity (e.g. [14]). Note that the narrowing of gaps occurs very rapidly. Parameters for the spectra in Fig. 1 are chosen so as to show that their structure for the graphene SL of different nature may be similar. The difference of two spectra is explained by that the velocity barriers are dependent on energy [9]. If we make an analogy between tunneling of quasi-particles in graphene through a rectangular electrostatic barrier and tunneling through a velocity barrier, for the potential of the last it is necessary to write down

$$U(E) = E - E/v_F, \tag{7}$$

in other words, expressions for the transmission coefficient T in the specified cases coincide if the condition (7) is satisfied. This formula explains the fact that spectra of $\mathrm{T}(E)$ for SL with the velocity barriers are periodic over all the energy scale. It is quite naturally that the expression for the transmission rates comprises the term that directly determines the spectra periodicity (see e.g. the recent papers [7,18,19]).

Note further that the graphene superlattices with the velocity barriers are characterized by a rich variety of the energy spectra, and also by their high sensitivity to minor changes in geometrical parameters of a lattice. This statement is correct in relation not only to quasi-periodically modulated SL, but to strictly periodic lattices as well and it allows for controlling the energy spectra in a wide range. In the general case, i.e. for arbitrary values of the parameter values the energy spectra demonstrate a set of irregularly spaced of allowed and forbidden bands. However for some sets of the parameter values spectra are regular and it is natural to take them for analysis in the first place; examples of such spectra

are shown in figures of this paper. (The same conclusion in relation to the strictly periodic SL with the velocity barriers was done in [18, 19]).
Apparently, depending on the parameters of the problem considered spectra may differ from each other significantly; they can reveal the simple form with the small minimal period equal to several energy units, but also they can expose much more complicated pattern of bands with the minimal period of several tens of energy units. Each set of values of parameters provides the original specter with its own minimal period and substructure. In the minimal period of each specter, there is a point with respect to which the specter is symmetric and besides each specter exhibits a symmetric substructure (e.g. Fig. 1).
Let us now consider some concrete energy spectra of the graphene Fibonacci SL modulated by the velocity barriers. Fig. 2 shows the trace map for the initial Fibonacci generations of the SL in which the quasi-periodic modulation is created due to different values of the velocity barriers, namely v_a=1, v_b=2, d=1, w=0.5, the energy range is selected to be the minimal period equal to 2π. The trace map investigated is characterized by the following features. For the taken set of parameters which corresponds to the trace map in Fig. 2, each Fibonacci generation forms spectra with a regular arrangement of the energy bands, and each of them exposes its own geometry. The higher generation is, the spectra of more complex pattern correspond to it. Note that spectra of higher generations are strongly fragmented (therefore we don't represent them), and besides fragmentation degree increases significantly with increase in geometrical SL parameters d, w.
With increasing the number of the Fibonacci sequence the number of gaps increases and their total width becomes larger. The fragmentation of the allowed bands in all generations starting from the third one occurs in accordance with the property of the self-similarity. Note also that, for some energy ranges, there are gaps in every Fibonacci sequence.
It should be noted further that in certain fixed energy areas, the Fibonacci inflation rule is satisfied: $z_n=z_{n-1}+z_{n-2}$, where z_n is number of bands in the n-th Fibonacci generation. The minimal such energy range is shown in Fig. 2. The numbers of the allowed bands in the consequent Fibonacci generations for the parameters chosen are 5, 8, 13, 21 for the 2-d, 3-d, 4-th and 5-th sequences respectively.
The main conclusion from the spectra presented is as follows: Fibonacci quasi-periodic modulation in graphene superlattices with the velocity barriers can be effectively realized by virtue of a difference in v_a and v_b values, i.e. in value of the velocity barriers (no additional factor is needed). And this fact is true for a case of normal incidence of quasi-electrons on a lattice. (Therefore, the statement of authors of [13] that in graphene-based SL (in contrast to other SL), the quasi-periodic modulation can be "manifested only at oblique incidence" of the Weyl-Dirac electrons on a lattice isn't correct. As the results of this work demonstrate (and also results of previous works [12, 14, 15]) the implementation of the quasi-periodic modulation depends on a quasi-periodicity factor, and we see that if this factor is realized either due to different magnitude of the velocity barriers (as in this work), or by virtue of different values of gaps (as in [14, 15]), the quasi-periodic modulation takes place not only at inclined incidence of quasi-particles on a lattice but also at their normal incidence).

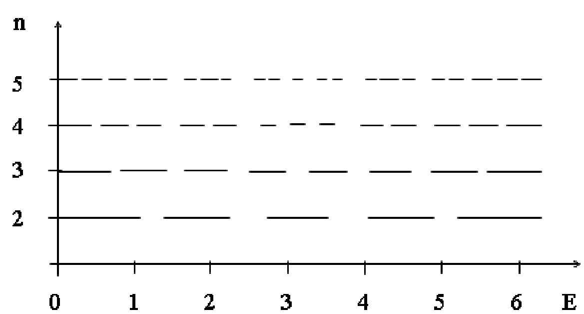
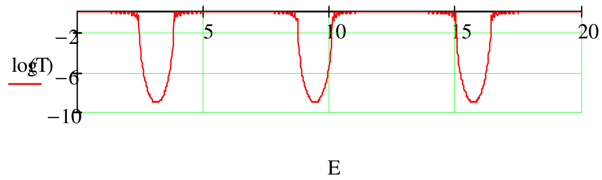


Fig. 2. Trace map for the initial Fibonacci generations, values of the parameters are as follows: d=1, w=0.5, v_a=1, v_b=2

We have shown above that the Fibonacci quasi-periodic modulation in the graphene SL can be created due to different Fermi velocity values in the SL barriers. There is another way to form an effective quasi-periodic modulation in the SL considered and it is due to different values of the electrostatic barriers in different elements of the array, while maintaining the velocity the same along the lattice chain. The external electrostatic potential U has a significant impact on the electron transmission and it is convenient to tune the transmission spectra with the help of this potential. Let us first consider briefly the effect of the external potential U on the strictly periodic SL with the velocity barriers. Denote the potential in elements *a* and *b* as U_a and U_b respectively; $U_a=U_b$ for the strictly periodic SL. The potential barriers are considered to be the piece wise constant, they are located along the SL chain (0x axis). The changes in the transmission spectra caused by the electrostatic potential are illustrated in Fig. 3 and are as follows: 1) a new (additional) gap appears between the two adjacent gaps which exist in the case of U=0; 2) a shift of all gaps is observed and it depends on the value of U; 3) the gap width depends on U also.



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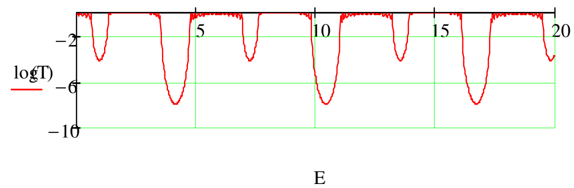

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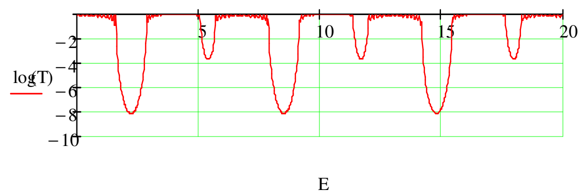


(c)

Fig. 3. Transmission spectra for the various values of the electrostatic potential U: U=0, U=2, U=4.5 for Fig. 3, a,b,c respectively, the other parameters: v_a=v_b=2, d=1, w=0.5

These changes are governed by the important property of the spectra – they are periodic with the potential U. For example for the parameters of Fig. 3 spectra return to their initial state at intervals δU=2πn, n – integer, i.e. the additional gap due to the external potential U doesn't appear. This means that for certain values of U the electrostatic barriers are perfectly transparent for the Dirac-Weyl quasi-electrons and thus there is a kind of the Klein paradox manifestation in the SL considered. (If v_a= v_b=1 we have T(E)=1 for all energies and values of U due to the Klein tunneling).The widening of gaps is accompanied by the narrowing of those gaps which relate to the SL with the velocity barriers for U=0.
The magnitude of the period oscillations δU can be found from the following considerations. According to the Bloch theorem we can write

$$\cos[\beta(d+w)] = 1/2\,\mathrm{Tr}(M_w M_a), \tag{8}$$

d+w is the lattice period. Calculation of the right side of this equation for the case of normal incidence of electrons yields the expression

$$\cos[\beta(d+w)] = \cos[(E-U)d/v \pm Ew], \tag{9}$$

v=v_a=v_b.

The last formula yields a value for the period of oscillations in the transmission spectra

$$\delta U = n\pi v/d. \tag{10}$$

This expression determines the dependence of the period δU on the SL geometric parameters (it is inversely proportional to the barrier width and holds for each value of the quantum well width) and on the Fermi velocity. Note that formula (10) holds well even for a small number of the SL periods.

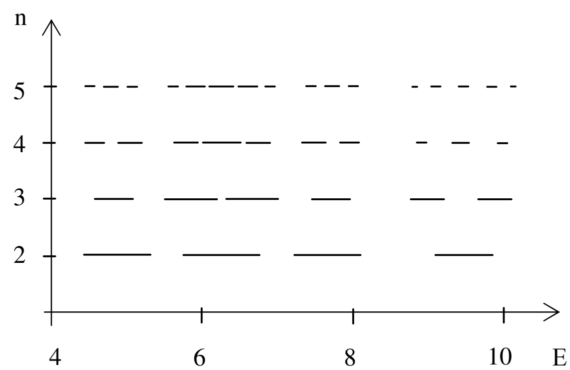


Fig. 4. Trace map for the initial Fibonacci generations of the SL with the parameters: U_a=0, U_b=π, v_a= v_b=2, d=1, w=0.5

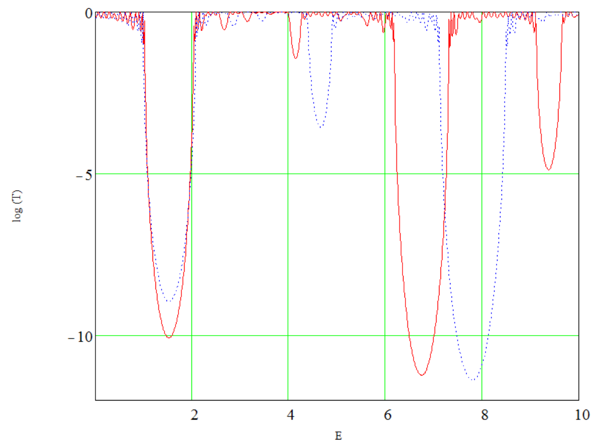
Fig. 4 shows a trace map for the SL under consideration for the difference $\Delta U=U_a-U_b=\pi$, other parameters as in Fig. 3, the energy interval is chosen to be equal to the minimal period in Fig. 3. In general, its character is similar to that plotted in Fig. 2 but some of its features must be noted here. This trace map is regular and gaps are wider than for other values of ΔU even if they are larger than π that is if the quasiperiodic factor is stronger. This is due to the fact that the spectra for the Fibonacci SL considered preserve the property of the periodicity in the case of $U_a \neq U_b$ and the factor of the quasi-periodicity is the secondary to the main property of periodicity. For values of $\Delta U=2\pi n$ the quasi-periodicity doesn't manifest itself at all and spectra repeat the initial state i.e. the one for U=0. The greatest splitting of the allowed bands is observed for values of ΔU slightly higher than πn. The trace map is not regular and symmetric for the arbitrary parameter values (for the general case when $U \neq \pi n$).
We see that the trace map in Fig. 4 is divided into two parts by the gap for energy equal to a little more than 8 (for ΔU chosen). The number of bands is subjected to the Fibonacci inflation rule in every part: for the initial Fibonacci generations we have the sequence of numbers 3, 4, 7, 11… and 1, 2, 3, 5… in the left and right parts respectively, and totally 4, 6, 10, 16… which differs from the case of Fig. 2.
Pay particular attention to the broad (lower energy) bands in each Fibonacci generation in Fig. 4. They correspond to the so called additional or superlattice Dirac bands in a periodic lattice [21]. It plays an important role in the controlling of the SL energy spectra since it is robust against the structural disorder. The location of the middle of such a band (mid-gap) E_D is determined by the condition [21]

$$q_d d + q_w w = 0 \tag{11}$$

which yields

$$E_D = Ud/(d + \upsilon\, w). \tag{12}$$

This equation for the position of the Dirac superlattice gap is well satisfied for a wide range of the parameters involved even for a small number of the SL periods. The Dirac band width depends on the problem parameters and may be less than the width of the other (Bragg) bands (see e.g. [14, 15,17]).
Similar Dirac superlattice gaps exist also in the case of the quasi-periodic Fibonacci SL investigated. The mid-gap position of such a gap may be approximately found by equation (13) (for not a large difference between U_a and U_b). Note further that a characteristic feature of the SL Dirac band is that it doesn't depend on the lattice period $d+w$, but it is sensitive to the ratio w/d. This is illustrated in Fig. 5 where log T(E) is plotted for the fourth Fibonacci generation with the parameters: v=2, U_a=4, U_b=3.5, the dashed line in Fig. 5a corresponds to values d=0.8, w=0.6, for the solid line d=0.96, w=0.72; for the solid line in Fig. 5b d=0.6, w=0.8, for the dashed line d=0.8, w=0.6.



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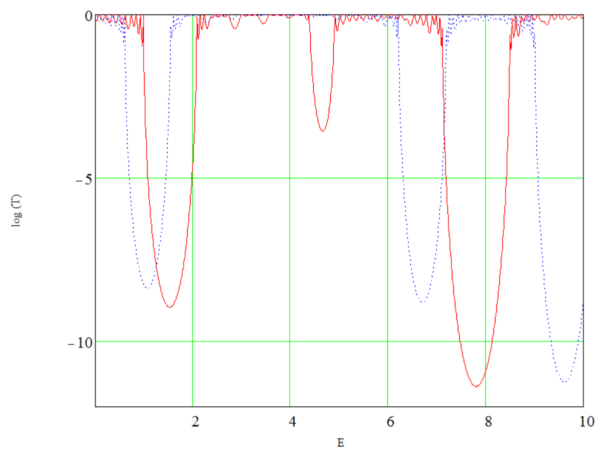

(b)

Fig. 5. Dependence of log (T) on energy *E* for the fourth Fibonacci generation, values of the parameters: v=2, U_a=4, U_b=3.5, the solid line in Fig. 5a corresponds to values d=0.96, w=0.72, for the dashed line d=0.8, w=0.6, for the solid line in Fig. 5b d=0.6, w=0.8, for the dashed line d=0.8, *w*=0.6

4. CONCLUSION

We analyze the energy spectra of the Fibonacci superlattice based on graphene modulated by the Fermi velocity barriers. The quasi-periodic modulation can be realized due to different values of the velocity barriers or due to different values of the external potential in the SL elements *a* and *b*. In contrast to the case of other types of the graphene SL spectra studied reveal the periodic character over all the energy scale and the transmission coefficient doesn't tend asymptotically to unity at rather large energies. The periodic dependence of the spectra considered on the magnitude of the external electrostatic potential is observed. Spectra demonstrate the rich variety of configurations (patterns) of the allowed and forbidden bands location dependent on one hand on the Fermi velocity magnitude and on the other hand on the SL geometry; for some special parameter values, they expose the regular character, symmetrical with respect to a certain point. The SL Dirac gaps are present in the spectra and their location depends on the velocity barriers value, on the value of the external potential as well as on the SL geometrical parameters. Results of our work can be applied for controlling the energy spectra of the graphene-based devices.

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