

Transmission Spectra of the Graphene-based Fibonacci Superlattice

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Abstract — We consider the gapped graphene superlattice (SL) constructed in accordance with the Fibonacci rule. We propose to create the quasi-periodic modulation due to the difference in the values of the energy gap in different SL elements. It is shown that the effective splitting of the allowed bands and thereby forming a series of gaps is realized under the normal incidence of electrons on the SL as well as under oblique incidence. Energy spectra reveal periodical character on the whole energy scale. The splitting of allowed bands is subjected to the inflation Fibonacci rule. The gap associated with the new Dirac point is formed in every Fibonacci generation. The location of this gap is robust against the change in the SL period but at the same time it is sensitive to the ratio of barrier and well widths; also it is weakly dependent on values of the mass term in the Hamiltonian. Results obtained allows for controlling the energetic spectra of the graphene-based superlattices and may be useful for operating of the nanoelectronic devices.

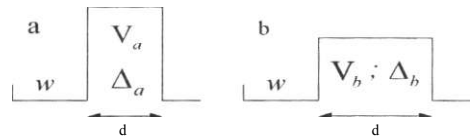
Keywords - *graphene-based superlattice; Fibonacci rule; transmission spectra*

I. INTRODUCTION

In recent years both graphene and graphene structures attracted much attention which is naturally explained by their non-trivial properties [1-3]. On the other hand, notable among the semiconductor structures including graphene ones are superlattices (SL) intermediate between periodic and disordered - quasi-periodic structures, e.g. Fibonacci, Thue-Morse and others. This is due to their unusual properties, such as self-similarity, fractal-like electronic spectrum etc. Attempts has already been started to study some kinds of superlattices based on graphene (Fibonacci and Thue-Morse [4-5]) which shed light on the behavior of Dirac chiral fermions in the quasi-periodic chains. Motivated by these circumstances, in this report we study the energetical spectra of the Fibonacci SL based 011 the monolayer gapped graphene. We propose to create the quasi-periodic modulation due to the difference in the values of the mass term A in the Hamiltonian in different elements of the superlattice. Because of the substantial progress in technology of graphene structures, in particular concerning the fabrication of the gapped graphene [6-9] we vary the value of A in wide range regardless of its nature which may be different [6-9].

II. METHOD OF EVALUATION

Consider the SL built of two elements "a" and "b".



Both elements contain the quantum well of width "w" and a potential barrier of width "d". The term A_n corresponds to the "a" element and the barrier height is denoted as V_n , for an element "b" we have A_n and V_n respectively. The SL is constructed according to the Fibonacci inflation rule. Thus for the fifth Fibonacci generation one can write : $S_5=abaababa$. The value of the transmission coefficient $T(E)$, E being the electron energy, through the SL built for a certain generation is determined by the period of this generation (sequence). Energy intervals in which the condition $T(E)=1$ holds form the allowed bands in energy spectrum, gaps are associated with values $T \ll 1$. The transmission coefficient can be evaluated by the transfer matrix method, by expressing T either in terms of the Green functions or the eigenfunctions. The latter are the solutions of the Dirac-like equation

$$[v_F(\mathbf{CT}, \mathbf{p}) + m \hat{v}_F^2 a_z + V(x) i] \cdot T = ET \quad (U)$$

where $v_F=10^6$ m/s, $\mathbf{p}=(p_x, p_y)$ the momentum operator $a=(\sigma_x, \sigma_y, \sigma_z)$ matrices for the pseudospin, $V(x)$

the external potential, which depends only on coordinate x , I - two-dimensional unit matrix, the mass term is denoted by the symbol A as adopted in the literature (units $c=h=v_F=1$ are adopted). The function H^T is a two-component pseudospinor $\Psi=[^1F_A, \Psi_B]^T$, $^1A, V_B$ are the envelope functions for the graphene sublattices A and B. Suppose that the potential consists of repetitive rectangular barriers along the x -axis and $V(x)=\text{const}$ within each j -th barrier. If we present solutions for the eigenfunctions T, B as a sum of plane waves traveling in the forward and backward directions of the x -axis then we obtain.

$$\langle P(x) = [a, \dots + b, -e \dots] \quad (2)$$

Transfer matrix connecting the wave functions at the points x and $x + Ax$ is found in several studies (see e.g.[1]) and has the form:

$$M_x = \begin{pmatrix} 1 - \cos(q_j \cdot Ax) & i Z_j \sin(q_j \cdot Ax) \\ \cos(q_j \cdot Ax) & -i Z_j \sin(q_j \cdot Ax) \end{pmatrix} \quad (3)$$

where $q_j = \sqrt{k_y^2 - k_x^2}$ if $k_x^2 > k_y^2$ and $q_j = k_x$ otherwise,

k_x is y-component of the wave number.

$$k_x = \text{sign}(s_j) [(E - V_j)^2 - A^2]^{1/2}, \quad s_j = s_j E - V_j(x) \pm A,$$

$$q_j = \text{sign}(s_j) \sqrt{k_x^2 - k_y^2} \quad \text{if } k_x^2 > k_y^2$$

and $q_j = k_x$ otherwise,

$$k_x = \sqrt{E^2 - V_j^2 - A^2}$$

the top line in (2) pertains to the sublattice A, the lower one - to the sublattice B.

The coefficient of the transmission of quasi-particles through the lattice $T = |t|^2$.

$$t = \frac{2 \cos \theta_0}{R}, \quad (4)$$

where θ_0 is the angle of incidence, and the matrix R is expressed as a product of matrices M_j :

$$R = \prod_{j=1}^N M_j$$

N - the number of elements in the SL.

III. RESULTS AND DISCUSSION

The trace map for 6 initial Fibonacci sequences is depicted in Fig.1 for the case where we have the gapped graphene in elements "a" and the gapless one in elements "b".

First of all it is noteworthy that the quasi-periodic modulation by setting different values of A in different SL elements used in this study results in the efficient splitting of the allowed energy bands and thus in the formation of a number of gaps. And this is realized at normal incidence of the electrons on the lattice.

Fig.2 exhibits the tunneling spectrum, i.e. the dependence of the transmission coefficient T on energy E for the 4-th Fibonacci generation under normal incidence of the electron wave on the lattice.

We see that the structure of some parts of the spectra is repeated periodically throughout the whole energy scale; one of these fragments of the spectrum can be considered as its period. The characteristic features of the period - the number of

allowed (forbidden) bands and their widths change so that with E increasing the gap's widths on average decrease. The natural result of this reduction is that the transmission coefficient asymptotically approaches to unity in the sufficiently far over-barrier region.



Fig. 1. Trace map for the Fibonacci SL, $k_y = 0, d = w = 0.5, V_A = V_B = 1, A_1 = L, A_0 = 0$.

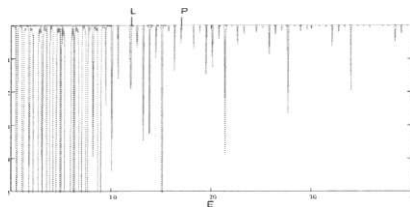


Fig. 2. Dependence of the transmission coefficient T on electrons energy E for the 4-th Fibonacci generation. values of the parameters: $k_y = 0, d = w = 0.5, V_A = V_B = 5, A_1 = L, A_0 = 0$.

The same spectrum in the energy range [0,6] is shown in Fig3.

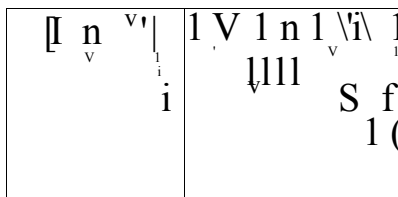


Fig. 3. Tunneling spectrum for the 4-th Fibonacci generation in the energy range [0,6]; values of the parameters are the same as those in Figure 2.

Spectra similar to that shown in Fig. 2 for the 4-th generation are observed also for other Fibonacci sequences.

The number of bands and the width of each of them depend on one hand on the SL parameters and on the other hand on the number of the generation.

As follows from the calculations, the number of allowed (forbidden) bands contained in one period, in particular in the interval CD in Fig. 3, corresponds to the Fibonacci sequence and this number is subjected to the Fibonacci inflation rule: $Z_{n+1} = Z_n + Z_{n-1}$, where n is the number of the Fibonacci generation (see Fig. 1). Note that this rule is applied not only to the CD period but to larger periods as well (e.g. LP in Fig. 2); every new super-period has its own number of bands.

As we can see in Fig. 1, 2, 3 at a certain energy all Fibonacci generations form the gap associated with the new Dirac point - "new Dirac point gap" [6]. Its location is almost unchanged in different Fibonacci sequences. A typical feature of the new Dirac point gap is that it is independent of the lattice period ($d + w$) and at the same time is sensitive to the ratio d/w . This is proved in particular by Fig. 4 which shows the dependence of T on E for the third Fibonacci generation for different values of w and d .

Once again we draw attention to the fact that the band's splitting (thereby forming a series of gaps) is realized even in the case of the normal incidence of electrons on the lattice surface.

IV. CONCLUSIONS

In summary, we have demonstrated that an effective quasiperiodic modulation can be achieved due to difference in mass term in different elements of the superlattice based on the monolayer graphene. The number of gaps within a period of the energy spectrum is subjected to the Fibonacci inflation rule.

The superlattice Dirac gap is observed in the spectrum and its features are analyzed.

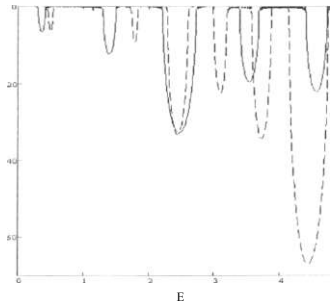


Fig. 4 Spectrum of the third Fibonacci sequence for different SL periods. $d=0.5$ (solid line), $d=1.1$ (dashed line), values of other parameters are the same as those in Figure 2.

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