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Discrete Solitons in the Bigraphene with Adsorbed Atomic Hydrogen

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Abstract—The propagation of discrete solitons in the bigraphene waveguides was calculated according to the Anderson model. An effective equation analogous to the classical sine–Gordon formula was obtained. The dependence of energy distribution between the waveguides of the graphene bilayers with adsorbed atomic hydrogen on the initial pulse width was studied.

Keywords: bigraphene, solitons, Anderson model, sine–Gordon equation.

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INTRODUCTION

There is currently growing interest in researching non-linear optical effects with the aim of incorporating them into practical devices [1]. The discovery of interesting new phenomena is thus expected owing to the unique properties of graphene and bigraphene [2, 3] when used as discrete waveguide structures for light propagation. We recently published a work that deals with spread of ultrashort optical pulses in carbon nanostructures [4, 5]. In this paper, we present our studies onthe propagation of solitary waves in bigraphene systems using the Anderson model.

STATEMENT OF THE PROBLEM AND BASIC EQUATIONS

To describe the electron spectrum of graphene [6], the Hamiltonian of Anderson's periodic model was written as follows:

$$H = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^{+} c_{k\sigma} + \sum_{\sigma} \varepsilon_{l\sigma} d_{l\sigma}^{+} d_{l\sigma} + U n_{l\sigma} n_{l-\sigma} + \sum_{lk\sigma} V_{lk} c_{k\sigma}^{+} d_{l\sigma} + \sum_{lk\sigma} V_{lk}^{*} d_{l\sigma}^{+} c_{k\sigma}, \quad (1)$$

where $c_{k\sigma}(c_{k\sigma}^{+})$ and $d_{l\sigma}(d_{l\sigma}^{+})$ are the creation and annihilation operators of electrons in a crystal and an atom, respectively; $n_{l\sigma}$ is the electron occupation number operator; $\varepsilon_{l\sigma}$ is the energy of a shell electron of an adsorbed atom (adatom); ε_k is the energy band of an electron in a crystal; V_{lk} is the matrix element of transition of electron from an adatom to graphene; and U is the energy of Coulomb interactions of electrons in an adatom.

Here we study a system consisting of several layers of bigraphene, a carbon nanostructure composed of double graphene sheets. We estimated the range of the problem and its major parameters in [7]. The system was considered in the tight binding model for πelectrons in the nearest neighbor approximation with interplanar hopping integral γ and an intraplanar hopping integral t_Δ of about 0.3 eV while electrostatic potential W was applied between the two layers of graphene. The full band structure of bigraphene described by the tight binding model in [8] allows us to write the Sombrero dispersion law in the form

$$E_{ps_k}^{\pm\pm}(W) = \pm\sqrt{E(k)^2 + t_\Delta^2/2 + W^4/4 \pm \sqrt{t_\Delta^4/4 + \left(t_\Delta^2 + W^2\right)E(k)^2}}. \quad (2)$$

where the plus and minus symbols refer to conduction and valent bands.

Let us consider an electromagnetic pulse with its wave vector propagating along bigraphene layers and its polarization vector being parallel to planes of bigraphene.

With regard to Coulomb calibration and allowing for the dielectric and magnetic properties of the system in [9], Maxwell's equation

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t},$$

could be written as:

$$\frac{\partial^2 \vec{A}_k}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 \vec{A}_k}{\partial t^2} + \frac{4\pi}{c}\vec{j}_k - \frac{4\pi}{c}\frac{\partial \vec{P}_k}{\partial t} = 0. \quad (3)$$

where $\vec{A}_k$ is the vector potential of the electromagnetic field in kth bigraphene layers $\vec{A}_k = (0, 0, A_k(x,t))$. $\vec{j}_k$ is the current flowing through the kth bigraphene layers, and $\vec{P}_k$ is the polarization induced by the electromag-

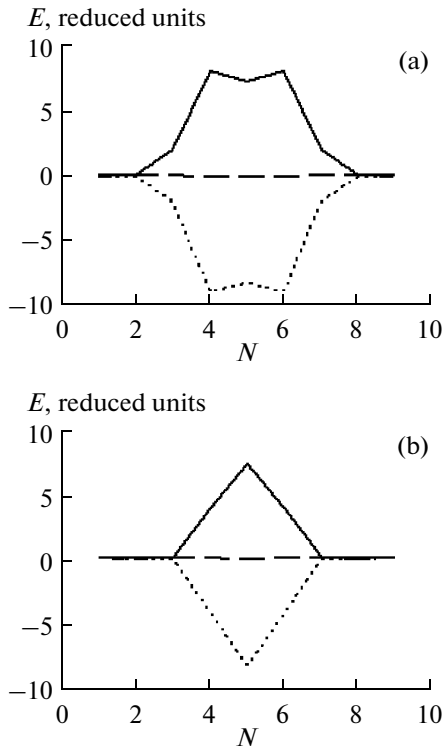

Fig. 1. Dependence of electric field values (E) on waveguide number (N) at (a) $\beta = 1$ and (b) $\beta = 3$ (all variables are dimensionless; 1 reduced unit of energy E and time t correspond to 10^8 V/m and 3×10^{-16} s, respectively; $W = 3$). Time values t are130, 200, and 260 for the solid, dotted, and dashed curves, respectively.

netic field in kth bigraphene layers and by the currents in adjusted layers of bigraphene. Furthermore, we restrict ourselves to a simple model where $\vec{P}_k = \alpha(\vec{E}_{ps_{k-1}} + \vec{E}_{ps_{k+1}})$, α is the coupling coefficient, and $\vec{E}_{ps_{k\pm1}}$ is the electric field values in the neighbouring layers of bigraphene.

The standard formula of the current density is:

$$j_k = e\sum_p \upsilon\left(p - \frac{e}{c}A_k(t)\right)\langle a_p^+ a_p\rangle, \quad (4)$$

where a_p^+ and a_p are the creation and annihilation operators of an electron with quasi-pulse p, $\upsilon(p) = \partial E_{ps_k}/\partial p$, and the square brackets denote the statistical average with respect to a nonequilibrium density matrix $\rho(t)$: $\langle B\rangle = \mathrm{Sp}(B(0)\rho(t))$.

Applying calculations similar to the one in [5], the formula for the current density in the system of bigraphene waveguides would be:

$$j_k = -en_0\sum_l D_l \sin\left(\frac{le}{c}A_k(t)\right),$$
$$D_l = \sum_{s=1}^{m}\int_{-\pi/a}^{\pi/a} dpB_{ls}\cos(lp)\frac{\exp\left(-E_{ps_k}(W)/k_BT\right)}{1+\exp\left(-E_{ps_k}(W)/k_BT\right)}, \quad (5)$$

where k_B is the Boltzmann's constant, T is the temperature, and the B_{ls} are coefficients in the Fourier series expansion of velocity of the charge carriers:

$$\upsilon_s(p) = \sum_l B_{ls}\sin(lp),$$
$$B_{ls} = \frac{1}{2\pi}\sum_p \upsilon_s(p)\sin(lp).$$

Equation (5) written in a dimensionless form therefore yields an analogue of the well-known sine–Gordon equation for when the generalized potential is expanded into a Fourier series:

$$\frac{\partial^2 R_k}{\partial x'^2} - \frac{1}{c^2}\frac{\partial^2 R_k}{\partial t'^2} - \mathrm{sgn}(D_1)\sin(R_k)$$
$$-\sum_{l=2}^{\infty}\left(\frac{D_l}{|D_1|}\sin(lR_k)\right) + \frac{4\pi\alpha}{c}\frac{\partial^2(R_{k-1}+R_{k+1})}{\partial t'^2} = 0, \quad (6)$$
$$R_k = \frac{eA_k}{c};\quad x' = x\frac{2e}{c}\sqrt{\pi n_0|D_1|};\quad t' = t\frac{2e}{c}\sqrt{\pi n_0|D_1|};$$

NUMERICAL SIMULATION

The studied equations were solved using the finite difference method with cross derivate terms. The initial pulse profile at the beginning of bigraphene waveguide system was chosen as:

$$R(t,N) = Ae^{-(t-t_0)^2}e^{-\beta(N-N_c)^2},$$

where A is the pulse amplitude, N_c is a number of the central waveguide ($N_c = 5$), β is the parameter defining the width of a pulse, N is the number of the waveguide, and t_0 is the initial time.

The dynamics of pulse propagation was studied in a system consisting of nine parallel bigraphene planes. The dependence of the electromagnetic field on a number of waveguides is shown in Fig. 1.

As can be seen from Fig. 1, pulse width β has a considerable effect on the distribution of energy between the waveguides. When $\beta = 1$, the energy thus reaches its maximum absolute values in waveguides no. 4 and 6 (Fig. 1a), while at $\beta = 3$ it is central (Fig. 1b). In addition, the inversion of signals occurs in the investigated system starting from a particular time based on the symmetry of the graphs.

Figure 2 shows that opposite the neighbouring waveguides, the shape of pulse in the central waveguide does not depend on the initial pulse width. The pulses in waveguides no. *5* and *6* thus have the same shapes, but lower amplitudes than the one in the central waveguide. The pulse weakens gradually with increasing distance from the central waveguide. By changing the initial pulse width at the central waveguide, it is therefore possible to control the

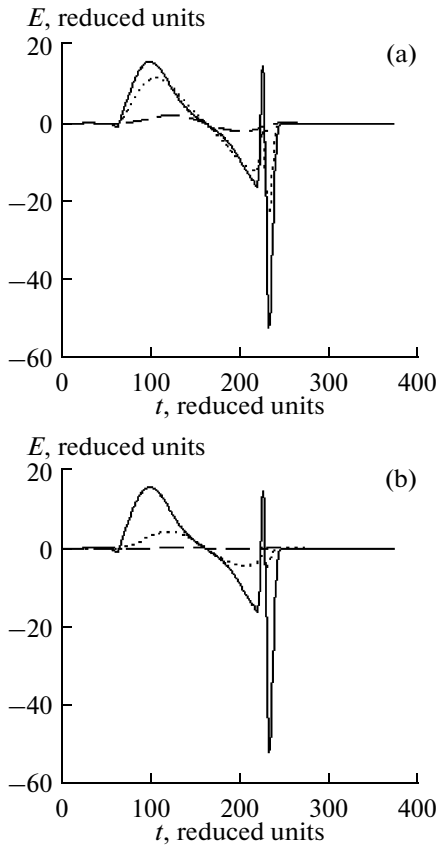

Fig. 2. Dependence of electromagnetic field values on time at (a) $\beta = 1$ and (b) $\beta = 3$ (all variables are dimensionless; 1 reduced unit of energy and time correspond to 10^8 V/m and 10^{-16} s, respectively; $W = 3$). The number of waveguide N is 5, 6, and 7 for the solid, dotted, and dashed curves, respectively.

amplitude of the electromagnetic field in the adjusted waveguides.

CONCLUSIONS

It was found that the magnitude of electrostatic potential W has little effect on the propagation of an electromagnetic pulse (considering shape and amplitude) in a system of bigraphene waveguides, due presumably to the presence of adsorbed atomic hydrogen.

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