Solitary waves in a two-dimensional graphene-based superlattice

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Abstract. The article is about the features of the propagation of solitary electromagnetic waves in the two-dimensional graphene superlattice both in the collisionless mode and in the collision mode. The quasiclassical approach has been used, in which the law of the dispersion of charge carriers is determined by the approximation of the quantum mechanical calculations. The magnitude of the electric current has been calculated by using the classic kinetic Boltzman equation with the model collision integral in the constant relaxation frequency approximation. The effect of the high-frequency electric field and the nonadditivity of the energy spectrum on the propagation of a solitary electromagnetic pulse in the arbitrary directions inside a sample has been determined. The numerical simulation of the evolution of solitary electromagnetic pulses is performed by using the method of difference schemes.

1. Introduction

With regard to the active study of new semiconductor structures based on a graphene, it is interesting to study nonlinear optical phenomena in them [1-6]. Their relevance is associated with the possibility of using graphene structures as a working medium for generating solitary electromagnetic pulses (SEP) [1], which have an applied interest [7,8]. The possibility of SEP generation in one-dimensional superlattices (SL) based on a graphene (GSL)[9] has been studied [3]. Recently, some researchers have focused on the study of two-dimensional (2D) GSL [10-16]. The development of the idea of the formation of a one-dimensional GSL [9] to the 2D case has been carried out in [10-11], in which the effect of externalelectric fields on the transport properties of a 2D GSL has been investigated. For the same structure, the features of anisotropy of the absorption coefficient of an electromagnetic wave in the presence of a constant electric field for the case of quasi-classically strong electric fields are considered [12]. In [13], the possibility of propagation of electromagnetic pulses in 2D GSL in the collisionless approximation has been investigated and the soliton-electric current and charge entrained by the soliton during its propagation have been calculated. In this paper, we consider issues related to the propagation of SEP in a 2D GSL both in the collisionless mode and in the collision mode.
2. Analytical approach
The law of the dispersion of charge carriers in a 2DGSL on a striped substrate (figure 1) in the single-minizone approximation can be described by the following form [10]

\[ e(\vec{p}) = \pm \sqrt{\Delta_0^2 + \Delta_1^2 (1 - \cos(p_x d_1/h)) + \Delta_2^2 (1 - \cos(p_y d_2/h))}, \]  

\[ p_x, p_y \] are the components of the electron quasimomentum, \( d = a_1 + b_1 \) is the GSL period, and \( a_1 \) and \( b_1 \) are the cell widths of gapless and gap graphene, coefficients \( \Delta_0, \Delta_1 \) and \( \Delta_2 \) were numerically selected by solving the dispersion equation. The different signs are associated with the conductivity and valence mini-bands. The GSL energy spectrum is non-additive; therefore, there is a dependence of the motion of charge carriers along orthogonal directions, and it is nonparabolic, which determines the nonlinear dependence of the electron velocity on the quasimomentum and the nonlinear properties of such structures, which are already manifested in relatively weak fields. This nonlinearity leads to the possibility of propagation in this type of SEP structures [17].

![Two-dimensional graphene superlattice](image)

Figure 1. Two-dimensional graphene superlattice.

The evolution of nonlinear SEP can be described by the d’Alembert equation for the vector potential when collisions are taken into account

\[ \frac{\partial^2 \vec{A}}{\partial x^2} + \frac{\partial^2 \vec{A}}{\partial y^2} - \frac{1}{c^2} \frac{\partial^2 \vec{A}}{\partial t^2} + \frac{4\pi}{c} j_0(A_x, A_y) = -\frac{4\pi}{c} j_d(A_x, A_y), \]  

\( \vec{A}(\vec{r},t) \) is the vector potential of the field, \( V = c\chi^{-1/2} \) is the speed of the electromagnetic wave in the absence of electrons, \( \chi \) is the effective dielectric constant. The vector potential is related to the electric field strength \( \vec{E} = -(1/c)\partial \vec{A}/\partial t \) (Coulomb calibration of potentials is used). The electric current density is determined as

\[ \vec{j} = -e \sum n(\vec{p}) \vec{v}(\vec{p}) \left( \vec{p} + \frac{e}{c} \vec{A}(\vec{r},t) \right), \]  

\( n(\vec{p}) \) is electron distribution function, \( \vec{v}(\vec{p})=\partial \vec{E}/\partial \vec{p}, \partial \vec{E}/\partial \vec{p}_y \) is electron velocity. In the collisionless limit, from Eq. (3) we obtain \( \vec{j}_0(A_x, A_y) \). The value on the right side of Eq. (2) \( \vec{j}_d(A_x, A_y) \) is a nonlinear functional of the perturbation of the current density \( \vec{j}_0(A_x, A_y) \) when taking into account collisions. To find the carrier distribution function, we used the classical Boltzmann equation with a model collision integral in the approximation of a constant relaxation frequency (\( \nu = \text{const} \))

\[ \frac{\partial n(\vec{p})}{\partial t} - \frac{e}{c} \frac{\partial \vec{A}}{\partial t} \frac{\partial n(\vec{p})}{\partial \vec{p}} = -\nu(n(\vec{p}) - n_0(\vec{p})). \]  

Due to the significant non-parabolicity of the electron spectrum in GSL, the conduction current is generally a nonlinear function of the field and the Eq. (2) is nonlinear. Note that due to the
nonadditivity of the energy spectrum, the orthogonal components of the vector potential are interrelated, which significantly affects the evolution of the SEP in the GSL.

In the case where the characteristic plasma frequency is much greater than the frequency of relaxation $\nu$ in the framework of the adiabatic perturbation theory, we have the system of the equations describing the slow evolution of the amplitude and phases of SEP. This system allows us to estimate the characteristic time of transformation of SEP into a linear electromagnetic wave [18].

In the collisionless mode, the system of equations for the components of the dimensionless vector potential corresponds to the weak nonadditivity of the energy spectrum

$$
\frac{\partial^2 \varphi_x}{\partial t^2} - \frac{\partial^2 \varphi_y}{\partial x^2} - \frac{\partial^2 \varphi_z}{\partial y^2} + \sin \varphi_x (1 + \beta \cos \varphi_x) = 0,
$$

$$
\frac{\partial^2 \varphi_y}{\partial t^2} - \frac{\partial^2 \varphi_x}{\partial x^2} - \frac{\partial^2 \varphi_z}{\partial y^2} + \sin \varphi_y (1 + \beta \cos \varphi_y) = 0,
$$

(5)

$$
\varphi = e(A, d_1, A, d_2)/ch, \quad t = t \sigma / \sqrt{\kappa}, \quad \tilde{x} = x \sigma / c, \quad \tilde{y} = y \sigma / c, \quad \beta = 2B_{11}/B_{10}, \quad \sigma^2 = 2\pi N e^2 B_{10} d / a \sigma, \quad B_0 \text{ is the coefficients of the decomposition of the current density in the double Fourier series, } N \text{ is the surface concentration of the conduction electrons, and } a \text{ is the thickness of the graphene layer.}
$$

If $\beta = 0$, then the connection between the orthogonal components disappears and Eq. (5) represent the well-known two-dimensional sine-Gordon equation.

Taking into account the symmetry of Eq. (5) and setting the symmetric initial conditions, we can obtain an equation describing the propagation of SEP at the angle of 45° to the GSL axes

$$
\frac{\partial^2 \varphi}{\partial t^2} - \frac{\partial^2 \varphi}{\partial x^2} + \sin \varphi + \frac{\beta}{2} \sin(2\varphi) = 0,
$$

(6)

$$
\bar{t} = \tilde{t} / \sqrt{2}. \quad \text{Eq. (6) is a double sine-Gordon equation which kink solution is well known [19, 20].}
$$

When collisions are taken into account, the right side of the Eq. (6) is modified and a nonlinear functional of the vector potential appears instead, expressed via a dissipative current

$$
\hat{R}[\varphi] = \gamma \int_{-\infty}^{\infty} d\tilde{t} \exp(-\gamma(\tilde{t} - \bar{t})) \{ \sin(\varphi(\tilde{t}) - \varphi(\bar{t})) + \lambda \sin(2(\varphi(\tilde{t}) - \varphi(\bar{t}))) + \\
+ \sin \varphi(\tilde{t}) + \lambda \sin(2\varphi(\tilde{t})) \} - \sin \varphi(\tilde{t}) - \lambda \sin(2\varphi(\tilde{t}))
$$

(7)

$$
\gamma = \nu \sqrt{\kappa} / \sigma, \quad \lambda = \beta / 2. \quad \text{If the functional is small enough, the problem can be solved using the adiabatic perturbation theory. The characteristic time of the wave evolution from essentially nonlinear to weakly nonlinear depends directly on the relaxation time, the square of the ratio of the stark and generalized plasma frequencies, and the nonlinear function of the parameter } \lambda. \quad \text{General methods of perturbation theory are then required. To increase the lifetime of the soliton, it is necessary to add energy using an external electric field or current.}
$$

To account for the ionization channel of the solitary wave attenuation, it is necessary first to determine the electron distribution function, which for this problem should be sought, taking into account the terms of generation and recombination of charge carriers in the Boltzmann kinetic equation. The electron distribution function is described by the Boltzmann equation, for the collision term of which the Batnagar-gross-crook model was adopted, taking into account the generation and recombination processes

$$
\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f = -\nu f - \frac{n}{n_0} f_0 + G(p, t) - \nabla (f - f_0).
$$

(8)

When solving Eq. (8), we obtain the expression for the distribution function, then find the current density and the nonlinear perturbation functional in the wave equation, which takes into account both impurity ionization and dissipation. The ionization current is expressed in terms of the
probability of ionization, which is convenient to find by the imaginary time method in the quasi-classical strong fields [12,14].

3. Numerical simulation

For the numerical simulation, we consider a special case corresponding to a symmetric SL $d_1 = d_2 = d = 2 \cdot 10^{-6}$. As a result of the numerical calculations, we obtain the following values: the approximation coefficients are $\Delta_0 = 0.4217 \Delta (\Delta = 0.13 \text{ eV}), \Delta_1 = \Delta_2 = 0.3318$; the width of the forbidden band between the valence and conductivity mini-bands is $\varepsilon_g = 0.8573 \Delta$; the width of the forbidden band between the first and second conductivity mini-bands $\varepsilon_{g12} = 0.6270 \Delta$; the width of the first conductivity mini-band is $\varepsilon_e = 0.2111 \Delta$.

The nonlinear wave Eq. (2) is generally solved numerically using the method of difference schemes. The system of Eqs. (2,5) has been solved numerically using a direct difference scheme of the "cross" type. The time and coordinate steps have been determined from some standard stability conditions. The steps of the difference scheme had been sequentially reduced twice until we reached the required accuracy.

Figure 2. The evolution of the electromagnetic pulse (a) $\bar{t} = 0$, (b) $\bar{t} = 3$, (c) $\bar{t} = 7$.

Fig. 2 shows the results of modelling the initial stage of the evolution of SEP with a Gaussian field potential in 2D GSL. This solution is called a breather in the one-dimensional case, and a pulson - in the two-dimensional case. To demonstrate and analyze the process of momentum evolution, it is convenient to choose certain directions in space and to record changes in the potential and electric field along these directions. Fig. 3 shows the results of the study of changes in the shape of the electromagnetic pulse both for the collisionless mode and for the collision mode. The pulse amplitude decreases rapidly, so the main task is to increase its lifetime.

Figure 3. Pulse profile with $\bar{y} = 20$ (center section) (a) $\bar{t} = 0$, (b) $\bar{t} = 7$, solid line - no collisions, dash line - with collisions.
The decrease in the pulse amplitude during its propagation is associated with the distribution of the energy of the initial perturbation over the sample area, and the generation of surface waves. Also, a key role in the pulse damping is belongs to collisions of electrons with the lattice, which are described by the model integral of collisions in the approximation of a constant relaxation frequency (time) [21].

The results of the interaction of two pulses are of particular interest. In the system of Eq. (5), a perturbation in one direction due to a weak coupling manifests itself in even small potentials in the orthogonal direction and vice versa. In the structures with an additive spectrum, two solitons running along the SL axes in mutually perpendicular directions will propagate without distortion. In our case, the mutual influence of solitons on each other is clearly visible in the numerical experiment.

4. Conclusion
The equation describing the propagation of electromagnetic waves in 2D GSL in the collisionless approximation and in the collision mode has been obtained. The software package for the numerical solution of the equation by using the grid method has been developed. The system of equations describing the evolution of the SEP amplitude and phase has been obtained on the base of the adiabatic perturbation theory. Due to the nonadditivity of the energy spectrum, the orthogonal components of the vector potential are interrelated, and it significantly affects the evolution of the SEP in 2D GSL.

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