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Propagation of extremely short pulses in a graphene–boron nitride bilayer

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ABSTRACT

In this study we investigate the propagation of extremely short optical pulses in a thin film formed by a graphene grown on a boron nitride substrate. Conduction electrons of the system are described on the basis of the long-wavelength effective Hamiltonian in the case of low temperatures; the electromagnetic field being taken into account within the framework of the classical Maxwell equations. The time evolution of the pulse's shape for different speeds and maximum amplitudes of an extremely short pulse is analyzed.

1. Introduction

Recently there has been an increase in the number of studies of graphene grown on a substrate of hexagonal boron nitride [1–10]. This is due to the unusual properties of graphene in this case [11]. More specifically, this is due to the similarity of the crystal structure of graphene and h-BN, and also to the fact that the ionic character of the interatomic bonds in the h-BN leads to an absence of the "dangling" covalent bonds and charge traps on its surface [12]. In Ref. [12], it was found that the roughness of graphene on h-BN is much smaller than that of graphene on SiO_2, and that the charge fluctuations are smaller by two orders of magnitude. In general, the electronic characteristics of graphene on h-BN are essentially the same as that of a free graphene, but it is much easier and more convenient to explore (and use) a graphene on this substrate [12].

In this Letter we investigate the dynamics of an extremely short optical pulse passing through a two-layer structure of graphene–boron nitride.

2. Basic formalism

Let us consider a thin film of graphene on a boron nitride substrate. In the long-wavelength approximation we choose the basis $\{\phi_{g1}, \phi_{g2}, \phi_{nb1}, \phi_{nb2}\}$, where the wave functions correspond to the electrons localized on two different sublattices of graphene, and the two different sublattices of boron nitride, respectively. The Hamiltonian in this case can be written in the block matrix form [13]:

$$H(k) = \begin{pmatrix} 0 & k^* & 0 & t \\ k & 0 & 0 & 0 \\ 0 & 0 & \Delta & f^* \\ t & 0 & f & -\Delta \end{pmatrix} \equiv \begin{pmatrix} H_{11} & H_{12} \\ H_{11} & H_{12} \end{pmatrix}, \tag{1}$$

where t is the electron hopping integral between layers of graphene and boron nitride, Δ is the energy gap for boron nitride, $k = v_{fg}(k_x + ik_y)$, v_{fg} is the Fermi velocity in graphene, k_x and k_y stand for the electron momentum components, $f = v_{nb}(k_x + ik_y)$, and v_{nb} is the Fermi velocity in boron nitride. When the energy gap, Δ, in boron nitride is large in comparison with the electron energy—still in the long-wavelength approximation—the effective Hamiltonian can be written analogously to the bigraphene case [14], namely

$$H_{\text{eff}} \equiv H_{11} - H_{12}H_{22}^{-1}H_{21} = -\frac{1}{t}\begin{pmatrix} \Delta & -\frac{1}{t}f^*k^* \\ -\frac{1}{t}fk & -\frac{1}{t^2}|k|^2\Delta \end{pmatrix}. \tag{2}$$

This approximation represents a constraint to the value of electron momentum [14], which allows us to use the long-wave approximation. The Hamiltonian (2) is easily diagonalized and gives us the energy spectrum for the electrons

$$\epsilon(k) = \frac{1}{2}\left(\Delta\left(1 - v_{fg}^2\left(k_x^2 + k_y^2\right)\right) + \sqrt{\Delta^2\left(1 - v_{fg}^2\left(k_x^2 + k_y^2\right)\right)^2 + \frac{4v_{fg}^2 v_{fnb}^2}{t^2}\left(k_x^2 + k_y^2\right)^2}\right). \tag{3}$$

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We now consider the application of an external electric field, $\mathbf{E}(x,t) = (0, E(x,t), 0)$, which is, to be specific, directed along the y axis. In this study we use the gauge $\mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}$. Following the general quantum mechanics rule, we have to replace the momentum by the generalized momentum, namely $p \to p - eA/c$, where e is the electron charge. In this case, the effective Hamiltonian (2) can be rewritten as

$$H_{\text{eff}} = \sum_{p\sigma} \epsilon\left(p - \frac{e}{c}A(t)\right) a^{\dagger}_{p\sigma} a_{p\sigma},$$

where $a^{\dagger}_{p\sigma}$ and $a_{p\sigma}$ are the creation and annihilation operators for electrons with quasi-momentum p and spin σ.

Maxwell equations with account for the dielectric and magnetic properties of a topological insulator in a quasi-1D approximation can be written as [15]

$$\frac{\partial^2 \mathbf{A}}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 \mathbf{A}}{\partial t^2} + \frac{4\pi}{c}\mathbf{j} = 0, \tag{4}$$

where we neglect the diffraction spreading of the optical pulse in the direction perpendicular to the axis of propagation. The vector potential $\mathbf{A}$ is considered to have the form $\mathbf{A} = (0, A(x,t), 0)$, and the current is $\mathbf{j} = (0, j(x,t), 0)$. Let us write the standard expression for the current density:

$$j = e\sum_{p} v_y\left(p - \frac{e}{c}A(x,t)\right)\langle a^{\dagger}_{p} a_{p}\rangle, \tag{5}$$

where $v_y(p) = \partial\epsilon(p_x, p_y)/\partial p_y$, and the angle brackets denote averaging with the non-equilibrium density matrix $\rho(t)$, i.e. $\langle\mathcal{L}\rangle = \mathrm{Sp}(\mathcal{L}(0)\rho(t))$ for an arbitrary physical quantity $\mathcal{L}$. Keeping in mind that $[a^{\dagger}_{p}a_{p}, H] = 0$, the equations of motion for the density matrix give us the relation $\langle a^{\dagger}_{p}a_{p}\rangle = \langle a^{\dagger}_{p}a_{p}\rangle_0$, where $\langle\mathcal{L}\rangle_0 = \mathrm{Sp}(\mathcal{L}(0)\rho(0))$. Thus, in the expression for the current density we can use a number of particles, which follows from the Fermi–Dirac distribution.

Next we consider the case of low temperatures, when only a small area in momentum space around the Fermi level contributes to the sum in (5). Accordingly, we write the formula (5) in the form

$$j = e\int_{-\Delta}^{\Delta} \mathrm{d}p_x \int_{-\Delta}^{\Delta} \mathrm{d}p_y\, v_y\left(p - \frac{e}{c}A(x,t)\right). \tag{6}$$

The domain of integration in momentum in Eq. (6), measured by Δ, is determined by the conservation of number of particles:

$$\int_{-\Delta}^{\Delta} \mathrm{d}p_x \int_{-\Delta}^{\Delta} \mathrm{d}p_y = \int_{-\Delta}^{\Delta} \mathrm{d}p_x \int_{-\Delta}^{\Delta} \mathrm{d}p_y \langle a^{\dagger}_{px,py} a_{px,py}\rangle.$$

Finally the equation for the propagation of an ultrashort pulse can be written as

$$\frac{\partial^2 A}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} + \frac{4\pi}{c}\Phi(A) = 0, \tag{7}$$

where the function $\Phi(A)$ is determined by integration of Eq. (6). Typical dependence of the nonlinearity present in Eq. (7) on the value of the field A is shown in Fig. 1.

3. Results of the numerical analysis

For the numerical solution of Eq. (7), we have implemented an explicit difference scheme of hyperbolic equations [16]. Difference scheme steps in both time and coordinates where iteratively decreased twice until the solution became unchanged in the eighth decimal place. The initial condition is chosen in the form of extremely short pulse consisting of a single oscillation, namely

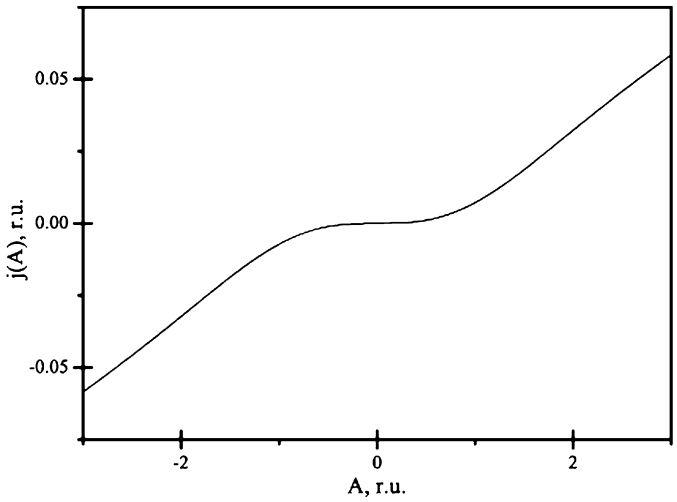

Fig. 1. The dependence of the current on the vector potential. All quantities are in dimensionless units.

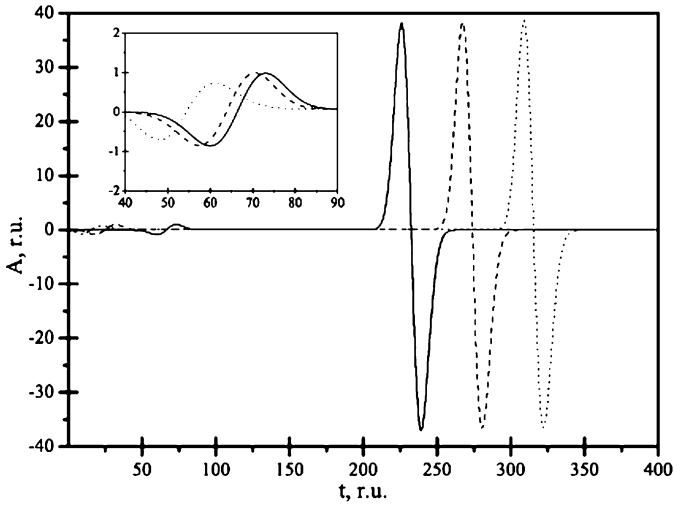

Fig. 2. The dependence of the pulse shape on the time for different points in space: (solid) $x = 10^{-5}$ m; (dashed) $x = 1.5\cdot 10^{-5}$ m; (dotted) $x = 2.5\cdot 10^{-5}$ m. The insert shows a close up for the early stage corresponding to t in the range 40 to 90 time units.

$$A(x,t) = Q\,\exp\left(-(x - vt)^2/\gamma\right), \tag{8}$$

$$\gamma = \left(1 - v^2\right)^{1/2}, \tag{9}$$

where Q is the amplitude, and v is the initial velocity of the pulse. This initial condition corresponds to the fact that the sample is irradiated with an extremely short pulse consisting of a single oscillation of the electric field. The energy parameters are expressed in units of Δ. The resulting evolution of the electromagnetic field propagating through the sample is shown in Fig. 2.

From Fig. 2, it appears clearly that the initial pulse splits into two parts. Moreover the smaller portion propagates in a direction opposite to the direction of the major one. The simplest model for this is that the pulse of the alternating electric field induces an alternating current in the system, which, in turn, induces an electric field interfering with the parental pulse. As a result of this interference, the initial pulse shape is not stable, and radiation of some energy occurs in the opposite direction. In other words, using an analogy with the theory of solitons [17], there is a decay of

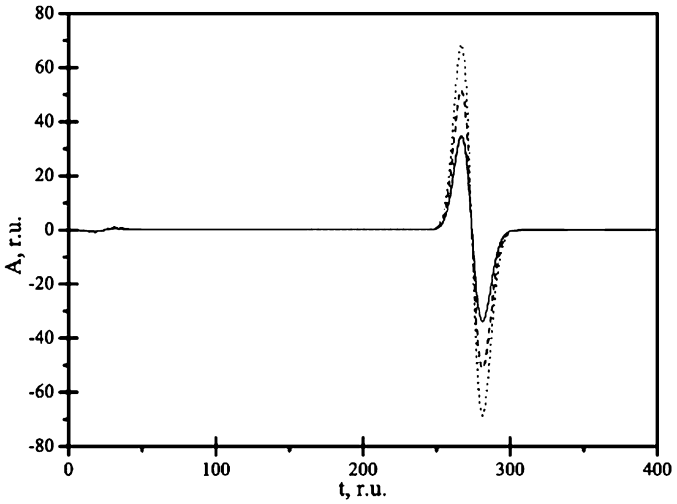

Fig. 3. Dependence of the pulse shape on the time for different values of the pulse amplitude: (solid) $Q = 3$; (dashed) $Q = 5$; (dotted) $Q = 7$.

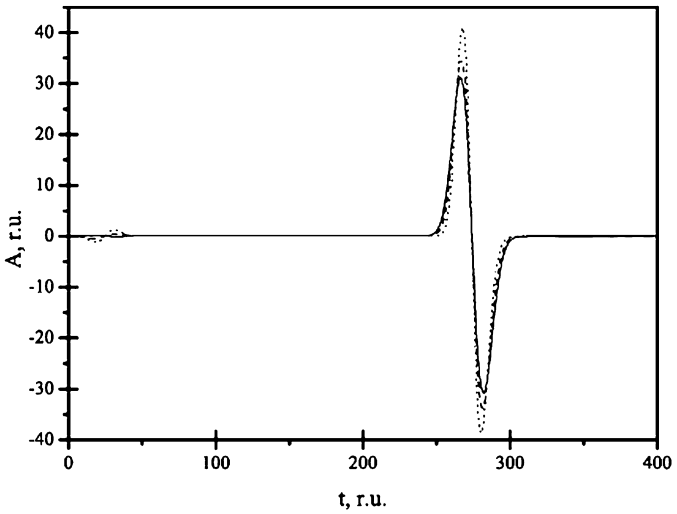

Fig. 4. Dependence of the pulse shape on the time for different values initial pulse speed: (solid) $v = 0.9$; (dashed) $v = 0.93$; (dotted) $v = 0.96$.

initially unstable pulse into two, each of which are stable due to a balance between dispersion and nonlinearity.

Such an interesting behavior is the outcome of two distinct effects at play in Eq. (7): (i) the linear part of Eq. (7), leading to a broadening of the optical pulse, as well as, (ii) the nonlinear term responsible for the narrowing of the pulse. The competition between these two effects leads to a deformation of the initial shape of the pulse and to the stabilization of its form. The effect of nonlinearity is even more pronounced when considering the dependence of the pulse shape on the initial amplitude, which is shown in Fig. 3. The pulse shape is extremely stable, which makes our system potentially useful in variety of applications.

The effects associated with nonlinearity manifest particularly strongly on the front of the pulse and lead, in particular, to the broadening of the pulse, that can be explained by an imbalance between the dispersion and nonlinearity in the system. Also note that the evolution of ultrashort pulses, in general, slightly depends on the speed of the initial pulse, which is shown in Fig. 4. This can be attributed to the Lorentz invariance of Eq. (7) and the effect of "squeezing" of the pulse when passing to a moving coordinate system.

4. Conclusions

The results obtained in this study show that the steady propagation of ultrashort optical pulses is possible in graphene grown on a substrate of hexagonal boron nitride. When the amplitude of the initial pulse increases, a weak broadening of the wave front takes place while a second pulse of lower intensity appears. This can certainly be useful in the development of hybrid devices based on the interaction of light with electrons in graphene.

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