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# Few-cycle optical pulses in a thin film of a topological insulator

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#### ABSTRACT

In this study we consider the propagation of few-cycle optical pulses in a thin film of a topological insulator. The electrons are described by means of the long-wavelength effective Hamiltonian at low temperatures, and the electromagnetic field is classically considered within the framework of Maxwell's equations. The time evolution of the pulse shape is analyzed for different values of its initial velocity and amplitude.

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The possible existence of topological insulators has been realized from studies of the quantum Hall effect in a confined two-dimensional electron gas [1]. In the case of the quantum Hall effect, the electrons move in a bounded region of space, staying away from the boundaries of the system, so that the sample is nonconductive. Near the boundaries (due to the "reflection" of electrons on the sample surface), an infinite motion is possible, or in other words, a current flow appears. This is due to the fact that in a magnetic field, electrons move along closed orbits, and the sample is an insulator. However, on the surface, electrons can be reflected from the boundaries, and a current flow becomes possible; its direction is determined by the electron spin and the magnetic field direction. Further investigations of this effect have entailed a transition from the interaction with an external magnetic field to the spin-orbit interaction [2,3], which eventually led to the discovery of the existence of topological insulators. Although there is an upsurge of research in this particular area, the question of the interaction of topological insulators with an intense external electromagnetic field has been overlooked-for instance, with the EM field consisting of extremely short optical pulses.

\* Corresponding author. Tel.: +65 86134730; fax: +65 67795161. *E-mail address:* alex\_zhukov@sutd.edu.sg (A.V. Zhukov). We consider a thin film of a topological insulator which, in the long-wave approximation and by taking into account the hexagonal warping of the Fermi surface, can be described by the following Hamiltonian [4,5]:

$$\mathcal{H} = \frac{p_x^2 + p_y^2}{2m} + v_F(p_x \sigma_y - p_y \sigma_x) + \frac{\lambda}{2} (p_+^3 + p_-^3) \sigma_z, \tag{1}$$

where  $p_{\pm} = p_x \pm p_y$ . The derivation of the effective Hamiltonian (1) for a thin film based on the Hamiltonian for a bulk sample is shown in several studies (e.g. Ref. [6]). Eq. (1) contains the components of the momentum,  $p_x$  and  $p_y$ , with the electron effective mass *m*, spin matrices  $\sigma_x$ ,  $\sigma_y$ , and  $\sigma_z$ , Fermi velocity  $v_F$ , and  $\lambda$  as the parameter related to hexagonal distortions. We use the typical values of the Hamiltonian parameters for Bi<sub>2</sub>Te<sub>3</sub> [4,5], namely  $m \sim 35 \text{ eV}^{-1}\text{\AA}^{-2}$  and  $v_F \sim 5 \times 10^{-4} \text{ eV}$ Å.

To be more precise in the construction of our model, it is worth noting that we considered the thin film of a topological insulator on a dielectric substrate. We neglected the substrate response at this stage of the investigation to demonstrate the possibility of a stable pulse propagation. The (linear and nonlinear) substrate response is beyond the scope of this paper and will be considered in future studies. The choice of such a simplified model is primarily dictated by the fact that the possibility of stable pulse propagation is due to the nonlinear dependence of the current on the applied field, the latter being determined by the properties at the surface of a topological insulator. After diagonalization, the Hamiltonian (1) gives the electron spectrum

$$\epsilon(p_x, p_y) = \frac{p_x^2 + p_y^2}{2m} + \sqrt{\nu_F^2(p_x^2 + p_y^2) + \lambda^2 p_x^2(p_x^2 - 3p_y^2)^2}.$$
(2)

Let us consider the electrical field directed along the *x*-axis using the canonical gauge  $cE = -\partial A/\partial t$ , where *E* is the electric field, and *A* stands for the vector potential. Following the general concepts of quantum mechanics, in the presence of an external electrical field we have to replace the momentum with its generalized counterpart,  $p \rightarrow p - eA/c$ , where *e* is the elementary charge. In this case, the Hamiltonian (1) can be recast as

$$\mathcal{H} = \sum_{p\sigma} \epsilon \left( p - \frac{e}{c} A(t) \right) a_{p\sigma}^{\dagger} a_{p\sigma}, \tag{3}$$

where  $a_{p\sigma}^{\dagger}$  and  $a_{p\sigma}$  are the creation and annihilation operators for electrons with quasi-momentum *p* and spin  $\sigma$ , respectively. Taking into account the dielectric and magnetic properties of the topological insulator and the gauge, Maxwell's equations in a quasi-1D approximation can be written as

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

where we neglect the diffraction spreading of the laser beam in the directions perpendicular to the axis of propagation. The vector potential and the current density are represented in the form A = (0, A(x, t), 0) and j = (0, j(x, t), 0), respectively. The current density can be written as

$$j = e \sum_{p} v_{y} \left( p - \frac{e}{c} A(x, t) \right) \langle a_{p}^{\dagger} a_{p} \rangle, \tag{4}$$

where  $v_y(p) = \partial \epsilon(p_x, p_y)/\partial p_y$ , and the brackets  $\langle ... \rangle$  stand for the average with the non-equilibrium density matrix  $\rho(t)$ , so that  $\langle B(t) \rangle = \operatorname{Sp}(B(0)\rho(t))$  (Sp denotes the matrix trace). Taking into account the commutator relation  $[a_p^{\dagger}a_p, \mathcal{H}] = 0$ , originating from the equations of motion for the density matrix, we obtain  $\langle a_p^{\dagger}a_p \rangle = \langle a_p^{\dagger}a_p \rangle_0$ , where  $\langle B(t) \rangle_0 = \operatorname{Sp}(B(0)\rho(0))$ .

Thus, in the expression for the current density, we can use the number of particles, which follows from the Fermi–Dirac distribution. Next, we consider the case of low temperatures, when the main contribution to the sum (4) comes only from a small region near the Fermi level in momentum space. Correspondingly, Eq. (4) can be recast as

$$j = e \int_{-\Delta}^{\Delta} \int_{-\Delta}^{\Delta} dp_x \, dp_y \, v_y \Big( p - \frac{e}{c} A(x, t) \Big). \tag{5}$$



**Fig. 1.** Vector potential versus time for different spatial points. All the quantities are scaled in relative units (r.u.). Curve (a) corresponds to  $x = 10^{-5}$  m, (b) to  $x = 1.5 \times 10^{-5}$  m, and (c) to  $x = 2 \times 10^{-5}$  m.

The domain of integration over the momenta in Eq. (5), i.e.  $\Delta$ , is determined from the conservation of the number of particles

$$\int_{-\Delta}^{\Delta} \int_{-\Delta}^{\Delta} dp_x \, dp_y = \iint_{BZ} dp_x \, dp_y \langle a_{p_x p_y}^{\dagger} a_{p_x p_y} \rangle$$

where *BZ* stands for the whole first Brillouin zone. The equation for the propagation of optical pulses can be written as

$$\frac{\partial^2 A}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2 A}{\partial t^2} + \frac{4\pi}{c} j(A) = 0, \tag{6}$$

where j(A) should be determined by integration in Eq. (5).

Eq. (6) is solved numerically using the direct difference scheme of the cross-type [8–10]. The time step and the spatial grid size are both determined from the standard conditions of stability. Difference scheme steps are iteratively decreased twice until the solution is unchanged in the eighth decimal place. The initial condition is chosen in the form of an extremely short pulse consisting of a single oscillation, namely

$$A(x,t) = B \exp\{-(x-vt)/\gamma\} \sin kx,$$
(7)

where  $\gamma = (1 - v^2/c^2)^{1/2}$ , *B* is the amplitude, *v* is the initial speed of the pulse, and *k* is the wavevector. 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  $\Delta$ . The resulting evolution of the electromagnetic field propagating through the sample is shown in Fig. 1. Note that this kind of behavior has not been observed previously. We believe that it is associated with the type of nonlinearity coming from the last term in Eq. (6). An asymmetry in the shape of the pulse is observed and is due to the fact that the front edge of the pulse and its trailing edge are in different conditions. Indeed, the electric field at the trailing edge of the pulse interferes with the electric field induced by the current, which arises during the passage of the front edge of the pulse.

The dependence of the pulse shape on the initial amplitude is shown in Fig. 2. As expected, low-amplitude pulses propagate almost without distortion, while still experiencing certain spreading due to the dispersion. Pulses of large amplitude experience greater distortion due to the interference effects between the leading edge of the pulse and its trailing edge, and by the characteristics of nonlinearity. Also, we have to note that the evolution of the extremely short pulse depends, in general, on the speed of the pulse at the entrance of the sample, as illustrated in Fig. 3. This behavior can be associated with the Lorentz-invariance of Eq. (6) and with the effect of "squeezing" of the pulse when passing to a moving coordinate system [7,11].



**Fig. 2.** Dependence of the pulse shape on time for different values of the pulse amplitude. All the quantities are scaled in relative units (r.u.). On curve (b), the pulse amplitude is 5 times larger than that for curve (a), while on curve (c), the pulse amplitude is 10 times larger than that for curve (a).



**Fig. 3.** Dependence of the pulse on time for different values of the pulse velocity at the inlet of the specimen. All the quantities are scaled in relative units (r.u.). Curve (a) corresponds to  $\nu = 0.9$ , (b) to  $\nu = 0.95$ , and (c) to  $\nu = 0.99$ .

One may be curious about our interest in the ultrashort pulse propagation, particularly in topological insulators, while there are lots of systems with nonlinearity. Indeed, soliton-type of pulse propagation has been demonstrated in a variety of low-dimensional systems (see, e.g. Refs. [10,12] and references therein). However, the influence of spin–orbit interactions is particularly pronounced in systems such as the one considered in the present study. So, we have demonstrated that this influence does not modify the dynamics with a proper choice of specimen parameters.

In conclusion, the results of our study demonstrate the possibility of stable propagation of few-cycle optical pulses in a thin film of a topological insulator. This effect may be useful in the development of hybrid devices based on the effects of the interaction of light with the electrons of a topological insulator. Note also that the effect associated with the formation of the "tail" of a very short pulse could be used to generate the terahertz pulses.

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