Edge absorption and pure spin current in a 2D topological insulator in the Volkov–Pankratov model

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Abstract
Light absorption due to transitions between the edge and two-dimensional (2D) states of a 2D topological insulator (TI) is considered in the Volkov–Pankratov model. It is shown that the transitions are allowed only for the in-plane electric field orthogonal to the TI edge. It is found that the absorption is accompanied by pure spin photocurrent along the TI edge. A possibility of spin current measurement using polarized luminescence from 2D TI quantum dots is discussed.

Keywords: 2D topological insulator, edge states, light absorption, pure spin current

1. Introduction
The main purpose of this paper is a study of the microwave absorption induced by the transitions from the edge states to 2D states of a 2D topological insulator. When the Fermi energy lies inside the energy gap and the microwave frequency is lower than the 2D absorption threshold, only these transitions are responsible for the absorption in a clean sample. Due to the rigid binding between the spin and direction of motion the absorption should be accompanied by the appearance of the edge spin current (for details see below).

The edge states in TI were the subject of numerous investigations [1–13]. Most of them rest on the so called Bernevig, Hughes and Zhang (BHZ) Hamiltonian [14] with zero boundary conditions and its generalizations. In our consideration we will base on the Volkov–Pankratov (VP) [1] model of the edge states of a 2D topological insulator. The VP model is a minimal model of border states in TI. It is based on the neglect of other energy bands, except for the two nearest ones which compose spin-degenerate valence and conduction bands. This determines the value of the model. Unlike the BHZ model, the edge functions in the VP model are non-zero both in an ordinary insulator (OI) and in TI.

The VP approach is valid if the distance to the other bands is longer than the OI gap. In a conventional BHZ model it is assumed that the 2D TI is surrounded by the OI (2D or 3D) impenetrable for electrons. The wave function in TI is supposed to satisfy the zero boundary condition on the TI border. This is not the case in the VP model.

In a real 2D HgTe the boundary between TI and OI is commonly formed as a result of etching. If the etching process is stopped too early, the HgTe layer would remain, but become thinner, at least nearby the intact 2D TI. (It is likely, this is done in real systems to avoid overetching; in any case this can be done intentionally.) In this situation the OI-TI border would be situated inside the QW. It is known that TI and OI differ in their quantum well (QW) widths $d$: $d > d_c$ for TI and $d < d_c$ for OI, where $d_c = 6.3$ nm. As a result, the border between OI and TI is given by relation $d(x, y) = d_c$. If the edge state width exceeds the 2D layer width one can neglect the vertical coordinate and study the problem as pure 2D one. Hence, below we will base on the 2D VP model of the edge states.

In the framework of the BHZ model of 2D TI the phototransitions and photogalvanic effect were studied in [15] (magnetodipole transitions between the edge states and electrodipole transitions between 2D states), [16, 17]
(electrodipole transitions between the edge and 2D bands). The magnetodipole transitions are very weak, while the electrodipole mechanism has been considered only for transitions near the Brillouin zone center.

Besides the absorption we will consider the non-equilibrium pure edge spin current described as a spin flow [18–20]. This current appears in systems with the spin–orbit correlation. Mathematically, this current is expressed via the symmetrized product of the operators of spin and velocity averaged with the density matrix.

The pure non-equilibrium spin currents were predicted and observed in a system with multiple GaAs quantum wells [21]. After this pioneering observation there were numerous studies of pure spin currents in different systems (see, e.g. [22–24]). However, nobody has studied this current in the edge states of topological insulator, where the tie of spin with the direction of motion is ultimate, so far.

Note that the interest to 2D TI edge states is supported by their most intriguing physical application to engineer [25, 26] Majorana fermions [27, 28] in systems where the 2D TI edge is adjoined to a superconductor. The localized Majorana zero-modes, obeying non-Abelian statistics, are perspective for quantum computing [29, 30]. Another direction [31–33] deals with superconductor–2D TI edge hybrid structures, where the edge plays the role of Josephson junction, and that reveals the intrinsic properties of TI edge states.

Thus, the potential applicability of the 2D TI edge states makes them to be an important object for exploration.

2. Electron states

In the 2D case the Hamiltonian of the VP model has the form:

\[ H = \begin{pmatrix} \Delta(x)\sigma_0 & i\sigma k_x \\ i\sigma k_x & -\Delta(x)\sigma_0 \end{pmatrix}, \]  

(1)

where \( k = (k_x, k_y) \) is the 2D momentum operator, \( \sigma_0 \) is the 2 \times 2 unit matrix, \( \sigma \) are Pauli matrices.

Below we consider a step-like dependence of \( \Delta(x) \) on the energy (11) with energies \( \varepsilon \). For a real \( k \) the energies get into the conduction and valence bands, respectively. The eigenfunctions are

\[ \psi^{(1,2)}_{k,\sigma} = \psi^{(1,2)}_{k,\sigma} e^{i(k_x x + k_y y)}, \]  

(3)

\[ \psi^{(1,2)}_{k,\sigma} = \psi^{(1,2)}_{k,\sigma} e^{i(k_x x + k_y y)}, \]  

(4)

\[ \psi^{(1,2)}_{k,\sigma} = \psi^{(1,2)}_{k,\sigma} e^{i(k_x x + k_y y)}, \]  

(5)

\[ \alpha^{(2)}_{k,\sigma} = \frac{\nu(k_x + i\sigma k_y^{(1,2)})}{E + \Delta_{1,2}}. \]  

(6)

The wave-functions of the Hamiltonian (1) localized near \( y = 0 \) are composed from the decaying waves with \( k^{(1,2)}_y = -i\lambda_{1,2}, \lambda_1 > 0 \) and \( \lambda_2 < 0 \) for \( y < 0 \) and \( y > 0 \), correspondingly. Using equation (2), we find \( \lambda_{1,2} = (\Delta_{1,2}^2 - E^2)/\nu^2 + k_y^2 \).

Continuity condition \( \Psi^{(1)}_{k,\sigma}|_{y=0} = \Psi^{(2)}_{k,\sigma}|_{y=0} \) yields edge states energies \( E = \varepsilon_{k,\sigma} \equiv \sigma v k_x \), parameters \( \lambda_{1,2} = \Delta_{1,2}/\nu \) and the localized edge eigenfunctions

\[ \Psi_{k,\sigma} = \frac{C \chi_{k,\sigma}}{\sqrt{\nu}} e^{i k_x x} \times \begin{cases} e^{i\frac{\Delta y}{2}} & \text{at } y < 0, \\ e^{-i\frac{\Delta y}{2}} & \text{at } y > 0, \end{cases} \]  

(7)

\[ \chi_{k_x,\sigma} = (1, 0, 0, 1), \]  

(8)

\[ \chi_{k_x,\sigma} = (0, 1, -1, 0), \]  

(9)

\[ C = \frac{1}{2} \sqrt{\frac{\Delta_1 |\Delta_2|}{\nu (\Delta_1 + |\Delta_2|)}}. \]  

(10)

These localized solutions are the only ones existing in domain \( |E| < |\Delta_2| \).

If \( \Delta_1 > |E| > |\Delta_2| \), in addition to the edge states, the 2D solutions appear delocalized at \( y > 0 \). Their wave-functions should decay at \( y \to -\infty \) and combine from the two propagating waves at \( y > 0 \) numerated by continuous momentum \( k_y > 0 \):

\[ \Psi_{k,\sigma} = e^{i k_x x} \times \begin{cases} C_{k,\sigma} e^{i k_y y} & \text{at } y < 0, \\ C_{k,\sigma} e^{-i k_y y} & \text{at } y > 0, \end{cases} \]  

(11)

Here \( \lambda = \sqrt{(\Delta_1^2 - \Delta_2^2)/\nu^2 + k_y^2} \). The continuity of the wave function at the interface gives

\[ C_{k,\sigma}^{(2)} = b_{k,\sigma} C_{k,\sigma}^{(1)}, \]  

(12)

\[ b_{k,\sigma} = \frac{\alpha_{k,\sigma}^{(2)} - \alpha_{k,\sigma}^{(1)}}{\alpha_{k,\sigma}^{(2)} - \alpha_{k,\sigma}^{(3)}}, \]  

(13)

where \( \alpha_{k,\sigma}^{(2)} \) is defined by equation (6) with \( E = \nu \varepsilon_k \equiv \nu \sqrt{\Delta_2^2 + \nu^2 k_y^2} \).

Normalizing the wave-function (11) we get

\[ C_{k,\sigma}^{(1)} = \left| 2 L \right| b_{k,\sigma} |2 + |\alpha_{k,\sigma}^{(2)}|^2 \right|^{-1/2}. \]  

(14)

The total energy spectrum is depicted in figure 1.
3. Probability of direct optical transitions and light absorption

The probability of direct transitions between edge and bulk states induced by the classical alternating electric field $E \cos (\omega t)$ is given by the matrix elements of electron velocity operator $V = \nabla_{\mathbf{k}} \mathcal{H}$. With the use of wave-functions equations (11) and (7), we get:

$$\langle V \rangle_{\nu, \mathbf{k}, \sigma, \mathbf{k}', \sigma'} = -2i\hbar^{2} C_{\mathbf{k}, \sigma}^{(1)} C$$

$$\times \frac{(\Delta_{1} + |\Delta_{2}|)(\nu \varepsilon_{k} + \varepsilon_{k, \sigma} + \Delta_{1} + \nu \lambda)}{(\varepsilon_{k, \sigma} + \nu \lambda)(\nu \varepsilon_{k} + \varepsilon_{k, \sigma})(\Delta_{1} + \nu \lambda)}.$$

According to equation (15) the $x$-component of the electric field is not absorbed. The probability of optical transitions caused by $E_{y}$ component of the electric field is

$$W_{\nu, \mathbf{k}, \sigma, \mathbf{k}', \sigma'} = \frac{\pi e^{2}}{2\omega^{2}} \theta^{2} (\varepsilon_{k} - \nu \varepsilon_{k, \sigma} - \omega)$$

$$\times |\langle V \rangle_{\nu, \mathbf{k}, \sigma, \mathbf{k}', \sigma'} E_{y}^{2}|^{2}. \quad (17)$$

The light absorption power per unit edge length $Q$ is expressed via the transition probabilities equation (17): 

$$Q = \frac{\omega}{L_{y}} \sum_{\nu, \mathbf{k}, \sigma} G_{\mathbf{k}, \sigma}^{(\nu)} \equiv \sum_{\nu} g_{\nu} \omega,$$  

where the generation rates in the transitions from the edge states to conduction band $G_{\mathbf{k}, \sigma}^{(\nu + 1)}$ and from the valence band to edge states $G_{\mathbf{k}, \sigma}^{(-1)}$ are

$$G_{\mathbf{k}, \sigma}^{(\nu + 1)} = W_{\nu + 1, \mathbf{k}, \sigma, \mathbf{k}', \sigma'} (\varepsilon_{k, \sigma}) \left(1 - f(\varepsilon_{k})\right), \quad (19)$$

$$G_{\mathbf{k}, \sigma}^{(-1)} = W_{\nu, \mathbf{k}, \sigma, \mathbf{k}', \sigma'} (\varepsilon_{k, \sigma}) \left(1 - f(\varepsilon_{k})\right). \quad (20)$$

Here $f(E)$ is the Fermi distribution function. At low temperatures and $|E_{F}| < |\Delta_{2}|$ ($E_{F}$ is the Fermi level) we have

$$G_{\mathbf{k}, \sigma}^{(\nu)} = W_{\nu, \mathbf{k}, \sigma, \mathbf{k}', \sigma} \theta (\nu \varepsilon_{f} - \varepsilon_{k, \sigma}). \quad (21)$$

Substituting $G_{\mathbf{k}, \sigma}^{(\nu)}$ from equation (21) into equation (18), after integration over $\mathbf{k}$ we get

$$g_{\nu} = g_{0} \frac{\delta^{2}}{\varepsilon_{f}^{2}} \left[ \eta_{\nu} \left( \eta_{\nu}^{2} - 1 \right) \left( \delta - \delta^{2} - \eta_{\nu}^{2} - 1 \right) \right]$$

$$+ \frac{\arctan \eta_{\nu} - \left( \delta - \delta^{2} - \eta_{\nu}^{2} - 1 \right)^{2} \arctan \left( \frac{\eta_{\nu} \delta}{\delta^{2} - \eta_{\nu}^{2} - 1} \right)}{\delta^{3} (\eta_{\nu}^{2} + 1)^{2}} \theta (\varepsilon_{f} - \varepsilon_{\nu}), \quad (22)$$

where $g_{0} = e^{2} E_{y}^{2} / (32 \pi \Delta_{1}^{2})$, $\delta = \Delta_{1} / |\Delta_{2}|$, $\varepsilon_{f} = \varepsilon_{\nu} / |\Delta_{2}|$, $\mu = E_{F} / |\Delta_{2}|$, $\varepsilon_{\nu} = \sqrt{\mu^{2} + 1 + \nu \mu}$, $\eta_{\nu} = \sqrt{\varepsilon_{f}^{2} - 2 \nu \mu - 1}$. The $\varepsilon_{\nu}$ thresholds correspond to the vertical optical transitions between the Fermi level and conduction or valence bands, correspondingly.

In the case of a trivial insulator with an infinite gap $\delta \rightarrow \infty$ we have

$$g_{\nu} \approx g_{0} \frac{\delta^{2}}{\varepsilon_{f}^{2}} \left( \frac{\arctan \eta_{\nu} - \eta_{\nu}}{\eta_{\nu} + 1} \right) \theta (\varepsilon_{f} - \varepsilon_{\nu}). \quad (23)$$

The edge absorption as the function of the frequency is shown in figure 2. Owing to the TI band symmetry, $Q(\mu) = Q(-\mu)$.

Note that the absence of the optical transitions caused by $E_{x}$ results from the e–h symmetry of the VP model. The same is valid in the BHZ model with $D = 0$, see [17].
We considered the homogeneous electric field. The presence of the electric field spatial dependence makes the intra-branch transitions caused by $E_x$ permitted [34]. However, the effect of the electromagnetic field inhomogeneity is rather weak due to the smallness of the external electromagnetic field wave vector. Nevertheless, if the edge is curved the acting effective electric field becomes strongly inhomogeneous. Similar situation have been studied for curved quantum wires of ordinary semiconductors, e.g. in [35–37].

Note, that the absorption exists near the boundary between a topological and an ordinary insulator. To observe the edge absorption, it is convenient to use an artificial structure with multiple edges, for example, with periodically alternating TI and OI domains, that can be done by the alternating quantum well width (see figure 3). In such a system the absorbing power will be proportional to the system area, instead of the edge length.

4. Spin current

Due to the topological protection, the electron spin number and the direction of motion conserve in the edge states. The phototransitions change the number of edge carriers. At the same time, the numbers of the left and right-moving carriers are equal. That means the absence of the edge photocurrent in the considered model.

Here we shall consider another effect: namely, the spin current. This quantity is determined by the mean product of spin and electron velocity operators \( \langle \sigma_i^j \rangle = \langle \hat{s}_i \hat{v}_j \rangle \). Topological protection makes edge carriers spin relaxation much longer than that of 2D carriers. Based on this fact we shall consider the contribution to the edge spin current only. In this approximation, the spin current flows within the TI edge states.

In a specific case of edge electrons and the optical excitation, the only spin current component \( (j_s)_{zx} \) exists. The velocity operator is reduced to $\sigma \hat{v}$. The product of spin number $\sigma$ and velocity, should be averaged with the non-equilibrium part of the distribution function of edge electrons $f_{\sigma,k_\nu}$. In the absence of backscattering, additional numbers of the particles excited to or from the edge states are conserved up to when carriers reach the contacts. In this ballistic regime all excited carriers contribute to the edge spin current. Hence, the ballistic current can be expressed via the total rate of carriers generation in edge states. The partial generation rate from the valence and to conduction bands differs in sign. Formally, we can write a kinetic equation

\[
\frac{\partial f_{\sigma,k_\nu}}{\partial x} = \sum_{\nu,k_{\nu}} G^{(\nu)}_{k_{\sigma}}.
\]

Solving the kinetic equation with the conditions $f_{\sigma,k_\nu}|_{x=-\pi L/2} = 0$ on contacts $\pm L/2$ we get the rate of spin pumping to the contacts:

\[
(j_s)_{zx} = -L \sum_{\nu} \frac{1}{4} \nu g_{\nu}, \tag{24}
\]

where $L$ is the distance between the contacts to the edge. Equation (24) shows that the spin current is proportional to the difference of the absorption contributions of the transitions from the valence band to the edge state and from the edge states to the conduction band. The dependencies of \( (j_s)_{zx} \) on the frequency and the Fermi level are shown in figure 4. The band symmetry yields \( (j_s)_{zx} (\mu) = - (j_s)_{zx} (-\mu) \).

The numerical estimations give the maximal value of \( (j_s)_{zx} = 6.5 \times 10^7 \) spins per second. We utilized quantities $E_x = 10$ V cm$^{-1}$, $\Delta_2 = -20$ meV, $L = 10^{-5}$ cm, $\nu = 5.5 \times 10^{10}$ cm s$^{-1}$.

**Figure 3.** A hypothetical structure for the edge absorption measurement. Wider HgTe layer parts represent TI, thinner part—OI.

**Figure 4.** Edge spin current (in units of $e^2 L^2/\Delta_2^2$) versus the dimensionless frequency $\varpi$ for different positions of the dimensionless Fermi level $\mu = 0, 0.2, 0.4, 0.6, 0.8, 1$ (the direction of $\mu$ growth is indicated by dashed arrow), $\delta = 0$. Thin arrows show the upper threshold $\varpi$ positions. Insert: Dependence $j_s(\mu) = -j_s(\mu)$ at $\varpi = 2$.

**Figure 5.** A sketch of hypothetic experiment for observation of the edge spin current. The front edge of a TI band is illuminated, the back edge is darkened. The spin current flow along the illuminated edge and collected by the TI quantum dots where stationary spin polarization occurs. The polarization can be measured, for example, via polarized luminescence.
Let us discuss the hypothetical experiment for the discovery of the edge spin current (see figure 5). To obtain the total edge spin current in the TI domain, one needs to break the symmetry between the opposite edges. This can be done if to illuminate only one edge leaving the other in darkness. The TI quantum dots connected to this edge will collect the spin and produce the opposite spin polarization of these dots. The spin polarization can be measured, for example, by the polarized luminescence from these dots. Practically, it would be more suitable to use the same 2D TI material for a large domain and spin-collecting quantum dots. The topological protection yields a long-living spin current in the TI domain, one needs to break the symmetry between the opposite edges. This can be done if to illuminate the TI dots in such a way that the number of pumped spins becomes comparable to the number of equilibrium carriers in TI dots in the large domain and spin-collecting quantum dots. The topological protection yields a long-living spin polarization both in the large domain and in TI dots. The small number of carriers in the edge states helps to reduce the number of equilibrium carriers in TI dots in such a way that the number of pumped spins becomes comparable to the number of equilibrium carriers. By a choice of the above-mentioned TI parameters, dot size $10^{-5}$ cm and spin relaxation time $10^{-6}$ s we hope to reach the spin polarization of dots up to 0.5.

5. Conclusions

We have calculated the edge absorption in a strip of 2D topological insulator due to the direct electrodipole transitions between the edge and 2D valence or conduction bands. The absorption is induced by the in-plane electric polarization normal to the edge direction. These phototransitions occur at illumination with frequency below the threshold of direct transitions in the 2D domain. Such absorption has been indirectly observed in the experiments on TI photoresponses [11]. We have found that the absorption is accompanied by the edge spin current. A possible way to measure the edge spin currents is offered.

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