Thin film of a topological insulator as a spin Hall insulator

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We study spin conductivity of the surface states in a thin film of a topological insulator with Kubo formulas. Hybridization between the different sides of the film opens a gap at the Dirac point. We found that in the gapped region spin conductivity remains finite. In the gapless region near the band gap spin conductivity is enhanced. These findings make a thin film of a topological insulator as a promising material for spintronic applications.

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Introduction. Spin Hall effect - generation of the transverse spin current by the applied voltage - have been predicted in the materials with spin-orbit scattering [1] and with strong spin-orbit interaction [2, 3]. However, it has been shown that spin current in latter materials is small due to vertex corrections caused by point disorder [4, 5], that is consistent with the experimental data [6].

While spin current is dissipationless itself [2], the accompanying charge current is dissipative. Ideal material for the spintronics should have high spin conductivity along with low charge conductivity. In fact, finite spin current can be produced in the thin film, where charge current is absent due to band gap. Such effect is referred as quantum spin Hall effect (QSHE) and it is predicted in narrow gap semiconductors [7], graphene with strong spin-orbit interaction [2, 3]. However, it has been shown that in the gapped region spin conductivity remains finite. In the gapless region near the band gap spin conductivity is enhanced. These findings make a thin film of a topological insulator as a promising material for spintronic applications.

Model. Low energy surface states in the thin film of topological insulator can be described by the Hamiltonian [16, 17, 20] ($\hbar = 1$)

$$H = r(k_x^2 + k_y^2) + \mu + v_F(k_x \sigma_y - k_y \sigma_x) \tau_z + \Delta \tau_x,$$

where $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices acting in the spin space, $\tau = (\tau_x, \tau_y, \tau_z)$ are the Pauli matrices acting in the layer space, $\mu$ is the chemical potential, $v_F$ is the Fermi velocity, $r = 1/(2m)$ is the inverse mass term, $s$ characterizes the next order correction to the Fermi velocity, $k_x = k \cos \phi$ and $k_y = k \sin \phi$ are the in-plane momentum components, $\Delta$ is the value of the gap at the Dirac point due to hybridization of the surface states belong to different layers. The spectrum of the Hamiltonian (1) is doubly degenerate and is given by

$$E_{\pm} = \mu + rk^2 \pm \sqrt{v_F^2 k^2 (1 + sk^2)^2 + \Delta^2}.$$  

If we measure the energy in terms of $v_F^2/r$, then, the chemical potential, the next order correction to the Fermi velocity, and the gap are conveniently characterized by the dimensionless values $r \mu/v_F^2$, $sv_F^2/r^2$, and $r \Delta/v_F^2$, respectively.

We obtain that the spectrum forms a Dirac cone when the Fermi velocity is large in comparison with the inverse mass term $sv_F^2/r^2 > 1/3$. Note, that vanished inverse mass term $r = 0$ leads to vanished spin conductivity.

In general, the spin conductivity can be presented as a sum of three terms [21, 22]

$$\sigma_{\alpha\beta}^\gamma = \sigma_{\alpha\beta}^{II} + \sigma_{\alpha\beta}^{III} + \sigma_{\alpha\beta}^{IV},$$

where the first two items correspond to a contribution from the states at the Fermi level and the third one from the filled states. Here $\alpha$ and $\beta$ denote the in-plane coordinates $x$ and $y$ correspondingly, and $\gamma$ denotes the spin projection.
At zero temperature \( \sigma_{\alpha\beta}^{\alpha\beta} \) and \( \sigma_{\alpha\beta}^{III} \) can be written in the form \[1, 21\]

\[
\sigma_{\alpha\beta}^{\alpha\beta} = \frac{e}{8\pi} \langle \text{Tr}[j_{\alpha}' G^+ V_{\beta} G^- - j_{\alpha}' G^- V_{\beta} G^+] \rangle, \tag{4}
\]

\[
\sigma_{\alpha\beta}^{III} = -\frac{e}{8\pi} \langle \text{Tr}[j_{\alpha}' G^+ V_{\beta} G^+ + j_{\alpha}' G^- V_{\beta} G^-] \rangle. \tag{5}
\]

Here \( j_{\alpha}' = \{\sigma_{\gamma}, v_{\alpha}\}/4 \) is the spin current operator, \( v_{\alpha} = \partial H/\partial k_{\alpha} \) is the velocity operator, \( \alpha, \beta \) is the momentum with vertex corrections, \( \{ \ldots \} \) means the anticommutator, \( \langle \ldots \rangle \) is for impurity average here and \( G^{\pm} \) are the retarded and advanced Green functions, which will be specified further.

The contribution to the spin conductivity from the filled states in a clean limit is \[3, 22\]

\[
\sigma_{\alpha\beta}^{III} = e \sum_{k, n \neq n'} (f_{n_{\alpha}k} - f_{n'_{\alpha}k}) \frac{\text{Im} \langle u_{n_{\alpha}k} | j_{\alpha}' | u_{n_{\beta}k} \rangle \langle u_{n_{\beta}k} | v_{\beta} | u_{n'_{\alpha}k} \rangle}{(E_{n_{\alpha}k} - E_{n'_{\alpha}k})^2}. \tag{6}
\]

Here \( E_{n_{\alpha}k} \) is the energy of an electron in the \( n \)-th band with the momentum \( k \), \( u_{n_{\alpha}k} \) is the corresponding Bloch function, \( \hat{H} u_{n_{\alpha}k} = E_{n_{\alpha}k} u_{n_{\alpha}k} \), \( f_{n_{\alpha}k} \) is the Fermi distribution function corresponding to \( E_{n_{\alpha}k} \) (which is the Heaviside step-function in the considered case of zero temperature), \( \text{Im} \) is for imaginary part, \( \langle \ldots \rangle \) is scalar production here.

**Spin conductivity from the filled states.** We start from the spin conductivity from the filled states given by the Eq. (6). Isotropic component \( \sigma^{III}_{xy} = -\sigma^{III}_{yx} \) is the only term that persists in the system. Using Eq. (6) we obtain

\[
\sigma^{III}_{xy} = \frac{e^2}{16\pi} \int \left( \theta(E_+) - \theta(E_-) \right) k \mathcal{D} k \frac{k^2 v_F^2 (2v_F^2 + \Delta^2)}{(v_F^2 + \Delta^2)^2}, \tag{7}
\]

where \( \theta(x) \) is Heaviside step function and \( \sigma_0 = e/(8\pi) \) is the spin conductivity quanta. Spin conductivity \( \sigma^{III}_{xy} \) is shown on the Fig. 2 for different values the the gap \( \Delta \) and Fermi velocity correction \( s \). Spin conductivity is a constant in the gapped region and decreases in the gapless. Also, its particle-hole asymmetry is controlled by the parameter \( s v_F^2/r^2 \): asymmetry smaller for larger values of the parameter. We can see that spin conductivity in a gapped region is comparable to the spin conductivity in a metallic region near the gap \( \sigma^{III}_{xy}(\mu = 0, \Delta) \approx \sigma^{III}_{xy}(\mu = \Delta, \Delta = 0) \), so at the Dirac point spin conductivity decreases with increase of the gap \( \Delta \).

**Disorder.** We will describe a disorder by a potential \( V_{\text{imp}} = u_0 \sum_i \delta(r - \mathbf{R}_i) \), where \( \delta(r) \) is the Dirac delta function, \( \mathbf{R}_i \) are positions of the randomly distributed point-like impurities with the local potential \( u_0 \) and concentration \( n_i \). We assume that the disorder is Gaussian, that is, \( \langle V_{\text{imp}} \rangle = 0 \) and \( \langle V_{\text{imp}}(\mathbf{r}_1)V_{\text{imp}}(\mathbf{r}_2) \rangle = n_i u_0^2 \delta(\mathbf{r}_1 - \mathbf{r}_2) \). We introduce disorder parameter as \( \gamma_0 = n_i u_0^2/(4v_F^2) \).

In the self-consistent Born approximation (SCBA), the impurity-averaged Green’s functions can be calculated as \( G^{\pm} = G_0^{\pm} + G_0^{\pm} \Sigma_{\mp} G^{\pm} \), where \( G_0^{\pm} \) are bare retarded/advanced Green’s functions of the Hamiltonian \( H \) and \( \Sigma^{\pm} \) is the self-energy. Self-energy is defined as \( \Sigma^{\pm} = \langle V_{\text{imp}} G^{\pm} V_{\text{imp}} \rangle \). In the case under consideration, we can calculate the self-energy \( \Sigma^{\pm} = S_{\mp} + i\Gamma \) using an Dyson equation \( \Sigma^{\pm} = n_i u_0^2 \sum_k G_{\mp}^{\pm} \). The self-energy has nontrivial structure in the layer space \( \tau \). Along with diagonal element \( \Sigma_0 \) it has non-diagonal one \( \Sigma_{\tau\tau} \). Therefore, the expression for \( G^{\pm} \) is similar to \( G_0^{\pm} \), in which \( \pm i0 \) is replaced by \( \pm i\Gamma \), \( \mu \) by \( \mu - \Sigma_0 \) and \( \Delta \) by \( \Delta - \Sigma_{\tau} + i\Gamma \).
The value $\Gamma_0$ describes interlayer scattering rate while $\Gamma_x$ describes intralayer scattering.

We start with the case of large chemical potential $|\mu| \gg \Delta$. In this case we can neglect a small correction to the value of $\mu$ due to real part of the self-energy and put $\Sigma' = 0$. In this limit we suppose that scattering rates $\Gamma_0, \Gamma_x \rightarrow 0$ are small and we obtain that $\Gamma = \text{Im}\Sigma = n_i u_0^2 \sum \text{Im}G_0^i$.

Now we consider scattering rate is independent of chemical potential and value of spin-orbit interaction $\\Gamma_0 = \gamma_0 |\mu|, \quad \Gamma_x = \gamma_0 \Delta |\mu|/|\mu| \quad (7)$

Condition $\Gamma_0 \Delta = \Gamma_x \mu$ stands even for $|\mu| \sim \Delta$. Near the band gap $|\mu| \sim \Delta$ we calculate scattering rates self-consistently and found that scattering rates are exponentially suppressed for a weak disorder $\Gamma_{0s}(x) \propto e^{-2/(\pi \gamma_0)}$ that is expected for the Dirac system [23].

The impurity averaged Green function can be calculated as $G^{\pm} = (1 + \Sigma G_0^a)^{-1} G_0^b$ or in the explicit form

\[
G^{\pm} = \frac{\mu + r k^2 \pm i \Gamma_0 - v_F k (x \alpha_y - y \alpha_x)}{\mu + r k^2 \pm i \Gamma_0} - \frac{v_F^2 k^2 + (\Delta \pm i \Gamma_x)^2}{(\mu + r k^2 \pm i \Gamma_0)^2} \quad (8)
\]

In the SCBA, following the approach described in Ref. [26], we can derive an equation for the vertex corrected velocity operator [27]

\[
V_\alpha(k) = v_\alpha(k) + \frac{n_i u_0^2}{(2\pi)^2} \int G^{+}(k)V_\alpha(k)G^{-}(k)d^2k. \quad (9)
\]

We found that $\Delta$ has a little influence on the vertex corrections. For $r = s = 0$ we get standard expression for the vertex corrected velocity operator $V_\alpha = 2v_\alpha$ [22, 27].

Point-like disorder renormalize $k$-independent part of the velocity operator. Thus, we write down

\[
\begin{align*}
V_x &= v_x + (v_F^{\sigma C} - v_F)\sigma_y, \\
V_y &= v_y - (v_F^{\sigma C} - v_F)\sigma_x,
\end{align*}
\]

where $v_F^{\sigma C}$ is calculated by the substitution of Eq. (10) into Eq. (9). Note, that some components in $V_\alpha(k)$ vanishes for the condition $\Gamma_0 \Delta = \Gamma_x \mu$.

Spin conductivity from the states at the Fermi surface. Now we use the obtained results and Eqs. (11) to calculate the contribution to the spin conductivity due to the states at the Fermi surface. On this way, we obtained, first, that in the considered approach the term $\sigma_{03,03}^{\sigma \gamma}$ vanishes exactly and we should compute the term $\sigma_{03,03}^{\sigma \gamma}$ only.

Isotropic tensor component $\sigma_{xy}^{Iz} = -\sigma_{xy}^{Iz}$ is the only term that exists in the system. From Eq. (11) using condition $\Gamma_0 \Delta = \Gamma_x \mu$ we derive

\[
\sigma_{xy}^{Iz} = \sigma_0 \int d k \frac{8 r \Gamma_0 v_F k (v_F^{\sigma C} + s k^2)}{\pi E_g + E_g - E_g} k^2, \quad (11)
\]

\[
E_g = (\mu + r k^2 + i \Gamma_0)^2 - v_F^2 k^2 - (\Delta \pm i \Gamma_x)^2.
\]
film enhances spin conductivity. This enhancement is cations. can be promising for a low dissipation spintronics appli-

absence of the states at the Fermi energy. Such phase
tering and dissipation is strongly suppressed due to an
flow of such bound states with zero charges will produce
the parent electron. If we apply electric field, then the
carries doubled spin and has spin-momentum locking of
same spin. Such bound state does not carry a charge but

electron (hole) from the Dirac cone of one layer to the

gap if we vary chemical potential. However, its
side the gap seems as an experimentally achievable
task.

To sum up, hybridization between the surface states in
different layers of thin films of topological insulators
opens a gap near the Dirac point. We found that finite
spin conductivity exists in the gapped region. In a metal-
ic region near the gap, spin conductivity is enhanced.
These findings can be crucial towards the implementation
of thin films of topological insulators in low-dissipation
spintronics.

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