Spin injection from topological insulator tunnel-coupled to metallic leads

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We study theoretically helical edge states of 2D and 3D topological insulators (TI) tunnel-coupled to metal leads and show that their transport properties are strongly affected by contacts as the latter play a role of a heat bath and induce damping and relaxation of electrons in the helical states of TI. A simple structure that produces a pure spin current in the external circuit is proposed. The current and spin current delivered to the external circuit depend on relation between characteristic lengths: damping length due to tunneling, contact length and, in case of 3D TI, mean free path and spin relaxation length caused by momentum scattering. If the damping length due to tunneling is the smallest one, then the electric and spin currents are proportional to the conductance quantum in 2D TI, and to the conductance quantum multiplied by the ratio of the contact width to the Fermi wavelength in 3D TI.

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Spin properties of edge and surface states of topological insulators (TI) are of great interest both for fundamental physics and for potential applications in spintronics [1]. The spin of electrons is strongly coupled to their momentum giving an idea of generating spin polarized currents in TI [2–4]. However, it would be interesting and of practical importance to generate not only spin polarized currents but pure spin currents as well. The general idea for generating pure spin current was suggested in Ref. [5]: a Y-shaped two-dimensional conductor forming a three-terminal junction with intrinsic spin-orbit interaction was proposed, where one of the terminals is a voltage probe which draws no electric current, but the polarizations of incoming and outcoming electrons are opposite to each other, causing a pure spin current. However, the particular realization of this system does not relate to TI. An example of a multiterminal system involving the edge state of TI, in which a pure spin current in the external circuit may occur is given in Ref. [6]. However, the decoherence and damping induced by contacts were out of consideration, while we find that damping and relaxation induced by coupling to a metallic contact are very important. The systems for generating a pure spin current suggested in Refs. [5, 6] were mesoscopic and ballistic. It is interesting to study a possibility to produce a pure spin current also in a 3D TI where the spin current can be larger as it is proportional to geometrical dimensions of the sample. In the helical surface state of 3D TI the physics is more complicated because a finite angle impurity scattering is not prohibited by momentum-spin locking and strongly affects transport properties.

In this paper we study an edge state in a 2D TI and a surface state in 3D TI coupled to metallic leads by tunnel contacts, take into account decoherence due to exchange of electrons with the lead and due to impurity scattering in 3D TI, and calculate charge and spin currents in the external circuit. A distinctive feature of our approach is that we take into account the decoherence induced by the contacts and show that it determines the electric and spin currents in the TI with contacts. We find that the currents strongly depend on relations between the characteristic lengths: the damping length due to tunneling, the length of the contact and the mean free path.

Below we set e, $\hbar$, and k_{B} to unity, restoring dimensional units in final expressions when necessary.

We consider a TI with a conducting helical state coupled by tunnel contacts to bulky leads (Figure) made of normal metal. The effects we study can be observed in various realizations but we consider the simplest three-terminal version when one of the leads is grounded, and the voltage V is symmetrically applied to the two other leads. We examine a 2D TI with the helical edge state (Fig. a) and a 3D TI cylinder with a conducting surface state (Fig. b). We denote the length of the tunnel contact to the grounded lead by l_0, while l_1 and l_2 stand for the lengths of the contacts to the leads with potentials $V_{\pm} = \pm V/2$.

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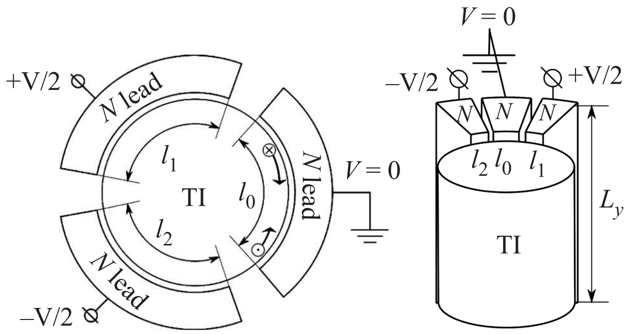

(a) – Helical edge state of 2D TI coupled to the leads. (b) – Helical surface state of 3D TI coupled to the leads

The total Hamiltonian reads

$$\hat{H} = \hat{H}_{\mathrm{TI}} + \sum_{i=1,2,3} \hat{H}_{\mathrm{lead},i} + \hat{H}_{\mathrm{tun},i}. \qquad (1)$$

Here $\hat{H}_{\mathrm{lead},i}$ is the Hamiltonian of the i-th lead, $\hat{H}_{\mathrm{TI}}$ is the Hamiltonian of the conducting state in TI. For the edge state [7–9]

$$\hat{H}_{\mathrm{TI}}^{(\mathrm{edge})} = \int dx \hat{\Psi}^{\dagger}(x) \left(-i\sigma_z v_{\mathrm{F}} \partial_x - \varepsilon_{\mathrm{F}}\right) \hat{\Psi}(x), \qquad (2)$$

where v_{F} is the velocity of the excitations, $\hat{\Psi}$ is a two-component spinor and $\boldsymbol{\sigma}$ are the Pauli matrices. We do not take into account impurity scattering in the 2D case, since spin-momentum locking prohibits such a scattering. For the surface state the Hamiltonian reads in the simplest case [8, 9]

$$\hat{H}_{\mathrm{TI}}^{(\mathrm{surf})} = \int d^2\mathbf{r}\ \hat{\Psi}^{\dagger}(\mathbf{r}) \left[(-iv_{\mathrm{F}}\partial_{\mathbf{r}} \times \mathbf{e}_z \cdot \boldsymbol{\sigma}) - \varepsilon_{\mathrm{F}} + \right. \\ \left. + V_{\mathrm{imp}}(\mathbf{r})\right] \hat{\Psi}(\mathbf{r}), \qquad (3)$$

where $\mathbf{e}_z$ is a unit vector perpendicular to the surface, V_{imp} is a random potential of impurities, and we assume that it is delta-correlated $\overline{V(\mathbf{r})V(\mathbf{r'})} = u_0\delta(\mathbf{r} - \mathbf{r'})$.

The tunnel Hamiltonian $\hat{H}_{\mathrm{tun}}$ reads

$$\hat{H}_{\mathrm{tun}} = \int d^3\mathbf{R} d^D\mathbf{r}\ \hat{\psi}^{\dagger}(\mathbf{R}) \mathcal{T}(R, r) \hat{\Psi}(\mathbf{r}) + \mathrm{h.c.}, \qquad (4)$$

where dimension $D = 1$ for the edge state and $D = 2$ for the surface state; $\hat{\psi}(\mathbf{R})$ is the field operator in a lead, the matrix element $\mathcal{T}(\mathbf{R}, \mathbf{r})$ describes tunneling between the lead and TI. We assume a site-to-site tunnelling which does not conserve momentum, $\mathcal{T}(\mathbf{R}, \mathbf{r}) = td^{(3-D)/2}\delta(\mathbf{R}_{\|} - \mathbf{r})\delta(\mathbf{R}_{\perp})$, where t is real and does not depend on $\mathbf{r}$, and $\delta(\mathbf{R}_{\perp})$ selects an average value of a function at a distance d of the order of inter-atomic scale near the surface.

First, we focus on the helical edge state coupled by tunnel contacts to the leads (Figure). We start from the Hamiltonian (1), (2), (4), and then derive equations for Keldysh matrices [10]

$$\check{G} = \begin{pmatrix} G^R & G^K \\ 0 & G^A \end{pmatrix}, \quad \check{\Sigma}_{\mathrm{tun}} = \begin{pmatrix} \Sigma^R & \Sigma^K \\ 0 & \Sigma^A \end{pmatrix},$$

where $G^{R,K,A}$ are Green functions of the edge state, Σ_{tun} is a self energy describing tunneling from a lead to the edge state. Deriving an expression for self energy we follow Kopnin and Melnikov [11]. For details one can also refer to Ref. [12], where the self energy was derived for helical states tunnel-coupled to a superconductor. Finally, we obtain $\Sigma_{\mathrm{tun}}(x, x') = \Sigma\delta(x - x')$, where

$$\check{\Sigma} = i\Gamma \begin{pmatrix} -1 & -2\tanh\dfrac{\varepsilon}{2T} \\ 0 & 1 \end{pmatrix}. \qquad (5)$$

Here we introduce the tunnelling rate $\Gamma \simeq \pi\nu_3 d^3 t^2 \sim t^2/\varepsilon_{\mathrm{F}}$, $\nu_3 = mp_{\mathrm{F}}/(2\pi^2\hbar^3)$ is the 3D density of states.

The Dyson equation for the Green functions $\check{G}$ reads

$$\left(\varepsilon + \varepsilon_{\mathrm{F}} + i\sigma_z v_{\mathrm{F}}\partial_x - \check{\Sigma}\right) \check{G}(x, x') = \delta(x - x'). \qquad (6)$$

The left-right subtracted Dyson equation for $G^K(x, x)$ can be reduced to a kinetic equation for distribution function f by ansatz $G^K = (G^R - G^A)(1 - 2f)$

$$\sigma_z v_{\mathrm{F}} \partial_x f = -\gamma(x)(f - f_i), \qquad (7)$$

where $\gamma = 2\Gamma/v_{\mathrm{F}}$ is the inverse damping length due to tunneling, $f_i = f_0(\varepsilon - V_i)$ is the equilibrium distribution function in the i-th lead.

Solving (6) for retarded and advanced components we obtain $G^R - G^A = -2\pi i\mathcal{N}(\varepsilon)$ where $\mathcal{N}(\varepsilon)$ is the density-of-states,

$$\mathcal{N}(\varepsilon) = \frac{\sinh\gamma l/2}{2\pi v[\cosh\gamma l/2 - \cos\left(k_{\mathrm{F}}L + \varepsilon L/v_{\mathrm{F}}\right)]}, \qquad (8)$$

where $l = l_0 + l_1 + l_2$ and L is the circumference of the edge state. In the limit $\gamma l \to \infty$ we obtain $\mathcal{N}(\varepsilon) \to 1/(2\pi v)$, and in the limit of small γl $\mathcal{N}(\varepsilon) \to \to \frac{1}{2v}\delta[\sin\left(\varepsilon + E_{\mathrm{F}}\right)L/2v]$.

The solution of (7) can be represented as a sum of equilibrium and non-equilibrium terms $f = f_0 + \delta f$. Non-equilibrium term at the region $0 < x < l_0$ coupled to the grounded lead reads

$$\delta f = \frac{\delta f_2 + [\delta f_1 - \delta f_2]\, e^{-\gamma\sigma_z l_2} - \delta f_1 e^{-\gamma\sigma_z(l_1 + l_2)}}{(1 - e^{-\gamma\sigma_z l})\, e^{\gamma\sigma_z x}}, \qquad (9)$$

where $\delta f_i = f_0(\varepsilon - V_i) - f_0(\varepsilon)$. The charge current flowing through the edge state is related to the non-equilibrium part of the Keldysh Green function G_{ne}^K by $I_e = \frac{i}{2}ev_{\mathrm{F}}\mathrm{Tr}\ \sigma_z G_{ne}^K$. Spin current reads $J_s = v_{\mathrm{F}}\rho$, where ρ is a linear density of electrons related to the

Keldysh Green function and a local shift of a chemical potential μ by equation $\rho = e\mu/(\pi v_F) - \frac{i}{2}\text{Tr}\ G^K_{ne}$. The local shift of a chemical potential μ is due to variation of electron density and obeys the Poisson equation $\left(\partial_x^2 + \partial_\perp^2\right)\mu = -4\pi e\rho\delta(\mathbf{r}_\perp)$. Finally, we obtain $J_s(x) \sim v_F\left(-\frac{i}{2}\text{Tr}\ G^K_{ne}\right)/(1+\alpha)$, $\alpha = ae^2/(\epsilon\hbar v_F)$, where $a \sim 1$ depends on the specific geometry, and ϵ is an ambient dielectric constant.

The spin current flowing through the grounded lead can be calculated as the difference of the spin currents in the edge state of TI at the endings of the contact $J_s = J_s(x=0) - J_s(x=l_0)$. Its derivative with respect to the applied voltage at low temperatures $T \ll \hbar v_F/L$ reads

$$\frac{dJ_s}{dV} = \frac{G_0}{e}\frac{4\pi v_F \sinh(\gamma l_0/2)\sinh(\gamma l_1/2)\sinh(\gamma l_2/2)}{(1+\alpha)\sinh(\gamma l/2)} \times \times \left[\mathcal{N}\left(\frac{V}{2}\right) + \mathcal{N}\left(-\frac{V}{2}\right)\right],$$

where $G_0 = e^2/h$ is the conductance quantum, and the density of states $\mathcal{N}$ is determined by Eq. (8). Here and below a spin current is measured in units of $\hbar/2$. In the limit of high temperatures $T > \hbar v_F/L$ the oscillations are washed out, and the term in the square brackets should be substituted by $1/(\pi v_F)$.

The electric current flowing through the grounded lead $I = I_e(x=0) - I_e(x=l_0)$ at low temperatures and in case of symmetrical geometry $l_1 = l_2$ is determined by conductance

$$\frac{dI}{dV} = G_0\frac{\pi v_F \sinh(\gamma l_0/2)\sinh\gamma l_1 \sinh(\gamma l_2/2)}{\sinh(\gamma l/2)} \times \times \left[\mathcal{N}\left(\frac{V}{2}\right) - \mathcal{N}\left(-\frac{V}{2}\right)\right]$$

that oscillates with the voltage and the Fermi level position (the latter can be varied by the gate voltage). At high temperatures $T > \hbar v_F/L$ and in the limit of large damping, $\gamma l_i \gg 1$, this term vanishes resulting in a pure spin current through the grounded lead.

It is instructive to consider an incoherent case $\gamma l_i \gg \gg 1$ in more details. In this case the non-equilibrium part of the electronic distribution at the region coupled to the grounded lead is reduced to

$$\delta f = \begin{pmatrix} \delta f_2 e^{-\gamma x} & 0 \\ 0 & \delta f_1 e^{\gamma(l_0 - x)} \end{pmatrix}. \tag{10}$$

Thus, due to the spin-momentum locking, the distribution of spin-up electrons at $x=0$ is determined by the heat bath coupled to the region $x<0$, and the distribution of spin-down electrons at $x = l_0$ is determined by the heat bath coupled to the region $x > l_0$. The spin current reads $J_s = [1+\alpha]^{-1}\frac{G_0}{e}V$ and the electric current equals zero, independent on the lengths of the contacts.

It is interesting that the electric current between the leads connected to a voltage source in the considered three-terminal structure equals $I = \frac{3}{2}G_0V$, and is different from the current in a two-terminal setup. In the latter case we find for the system with two tunneling contacts the same result $I = 2G_0V$ as in case of ballistic quantum wire attached to ideal adiabatic contacts.

Now we consider a surface state of a 3D TI tunnel-coupled to the leads (Fig. b). The Hamiltonian is given by (1), (3), (4). We assume that the contacts are placed on the (111) plane – in this case Pauli matrices in the Hamiltonian (3) coincide with the electron's spin operator [13]. The Dyson equation reads

$$\left[i\partial_t + \varepsilon_F + iv_F(\partial_y\sigma_x - \partial_x\sigma_y) - \check{\Sigma}_{\text{tun}} - \check{\Sigma}_{\text{imp}}\right]\check{G}(\mathbf{r},\mathbf{r}') = = \delta(\mathbf{r}-\mathbf{r}').$$

The self-energy for impurities $\check{\Sigma}_{\text{imp}} = -i\tau^{-1}\langle\check{g}\rangle$, where $\tau^{-1} = \pi\nu_2 u^2$, $\nu_2 = p_F/(2\pi\hbar^2 v_F)$ is the single-particle density of states at the Fermi energy and $\langle\check{g}\rangle$ is the average over the momentum direction of the quasiclassical Green function given by definition $\check{g} = \frac{i}{\pi}\int\check{G}d\xi$. Similarly to the case of tunneling into the edge state, the self-energy $\check{\Sigma}(\mathbf{r},\mathbf{r}') = \check{\Sigma}(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')$, and $\check{\Sigma}(\mathbf{r})$ is given by (5). The electron transport is determined by an interplay between three characteristic scales: the lengths of tunnel contact l_i, the damping length due to tunnel contacts v_F/Γ, and the momentum and spin relaxation length $v_F\tau$ due to impurity scattering. We focus on the case when the dimensions of the sample are larger than the mean free path and the dimensional quantization can be ignored. We follow Ref. [14] and obtain the kinetic equation for the distribution function f

$$\partial_t f + v_F(\mathbf{n},\nabla)f = -\frac{f - \langle f\rangle - (\mathbf{n},\langle f\mathbf{n}\rangle)}{\tau} - 2\Gamma(x)(f - f_i). \tag{11}$$

The distribution function f yields the quasiclassical Keldysh Green function by relation

$$g^K = (g^R - g^A)(1-2f) = (1 + n_y\sigma_x - n_x\sigma_y)(1-2f).$$

We represent the distribution function as a sum of isotropic and anisotropic terms, expanding angular dependence to the first harmonics $f \approx \langle f\rangle + f_x n_x + f_y n_y$, and the term with n_y vanishes due to translational symmetry along the y-axis. The electron and current density read

$$\rho = \frac{\nu_2}{2}\int\langle f\rangle d\varepsilon + \nu_2\mu, \quad j = \frac{v_F\nu_2}{2}\int f_x d\varepsilon.$$

Following Ref. [14] and taking into account a local shift of a chemical potential one can obtain from the kinetic equation (11) the continuity equation with the source describing tunneling, and the expression for the electric current

$$\partial_t \rho + \partial_x j = 2\Gamma(x)\left[\rho - \nu_2(\mu - V_i)\right], \qquad (12)$$

$$j = \sigma E + D\partial_x \rho, \qquad (13)$$

where V_i is a potential applied to the lead, $D = v_{\rm F}^2\tau/(1+4\Gamma\tau)$, $\sigma = e^2 v_{\rm F} p_{\rm F}/[2\pi(\tau^{-1}+4\Gamma-2i\omega)]$. The spin current density in the TI reads

$$j_s = v_{\rm F}\frac{\rho}{2}. \qquad (14)$$

However, spin relaxation due to scattering on impurities results in non-conservation of the spin current, and unlike the case of the edge state we cannot calculate the spin current flowing through the lead as the difference of the spin currents in the surface state of TI at the endings of the contact unless the contact length l_0 is shorter than the mean free path $\tau v_{\rm F}$. Thus, in order to calculate the spin current through the lead we use the continuity equation in the lead [14]

$$\partial_t \rho_s^{(\rm lead)}(x,y) + {\rm div}\, j_s^{(\rm lead)}(x,y) = \\ = \Gamma'(x)\delta(z)\rho_s^{(\rm lead)}(x,y) + 2v_{\rm F}^{-1}\Gamma(x) j_e^{(\rm TI)}(x,y)\delta(z), \qquad (15)$$

where $\Gamma' = \Gamma\nu_2/\nu_3$, ρ_s and j_s are spin and spin current densities in the lead, $j_e^{(\rm TI)}$ is particle current density in the TI. The term with ρ_s in the right-hand side vanishes in the leading approximation. Integrating (15) over space allows us to relate the spin current in the lead with the electric current in the TI

$$J_s = \frac{1}{v_{\rm F}}\int 2\Gamma j_e^{(\rm TI)} dxdy. \qquad (16)$$

Note that in the limiting case $\tau^{-1} \ll \Gamma$ according to (13), (14) expression (16) is reduced to the difference of the spin currents in the surface state of TI at the endings of the contact.

Now it is straightforward to calculate the spin current through the grounded lead using equations (12), (13) and demanding continuity of particle and current densities at the boundaries of the contacts. The result has especially simple form when $v_{\rm F}/\Gamma \ll l_i$:

$$J_s = \frac{G_0}{e} k_{\rm F} L_y \frac{1}{\left[4+(\Gamma\tau)^{-1}\right](1+s l_D)} eV,$$

where s is a spacing between contacts, $l_D = \sqrt{D/(8\Gamma)}$ is a diffusion length.

The electric current through the grounded lead equals zero. If the mean free path $\tau v_{\rm F}$ is greater than the damping length due to tunneling $v_{\rm F}/\Gamma$ then impurity scattering and corresponding spin relaxation do not affect spin current.

To summarize, we have proposed a system based on the 2D/3D TI which injects pure spin current into an external circuit. We have found that charge and spin transport is strongly affected by contacts connecting the TI to bulky leads which play a role of a heat bath. If the tunneling rate is large enough so that the exchange of electrons between the TI and the lead is intensive enough, the distribution functions of the electrons that passed the contact are determined by the Fermi distribution in the lead shifted by the applied voltage. This is somewhat similar to the case of quantum wire connected to the leads by ideal contacts, and similarly to the quantum wires yields electric and spin currents through a 1D channel being proportional to the conductance quantum. In case of 2D conducting region the current through the width of the order of the Fermi wavelength is proportional to the conductance quantum. Thus the conductance does not depend on the transmission of the contact if the tunnel coupling is not too weak, and the contact behaves as if it is nearly ideal. Though formally our results are valid in the tunneling limit only, we believe that they provide a qualitative description of the transport for any contacts.

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1. D. Pesin and A. H. MacDonald, Nature Materials **11**, 409 (2012).
2. S. Modak, K. Sengupta, and D. Sen, Phys. Rev. B **86**, 205114 (2012).
3. C. Brüne, A. Roth, H. Buhmann et al., Nature Physics **8**, 485 (2012).
4. A. A. Sukhanov and V. A. Sablikov, Journal of Physics: Condensed Matter **24**, 405301 (2012).
5. T. Pareek, Phys. Rev Lett. **92**, 76601 (2004).
6. F. Dolcini, Phys. Rev. B **83**, 165304 (2011).
7. M. König, H. Buhmann, L. W. Molenkamp et al., J. Phys. Soc. Jpn. **77**, 031007 (2008).
8. H. Zhang, C.-X. Lium X.-L. Qi et al., Nature Physics **5**, 438 (2009).
9. M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).
10. L. V. Keldysh, ZhETF **47**, 1515 (1964) [Sov. Phys. JETP **20**, 1018 (1965)].
11. N. B. Kopnin and A. S. Melnikov, Phys. Rev. B **84**, 064524 (2011).
12. T. D. Stanescu and S. Tewari, J. of Phys.: Condensed Matter **25**, 233201 (2013).
13. P. G. Silvestrov, P. W. Brouwer, and E. G. Mishchenko, Phys. Rev. B **86**, 075302 (2012).
14. P. Schwab, R. Raimondi, and C. Gorini, Europhysics Lett. **93**, 67004 (2011).