

Backscattering in a 2D topological insulator and conductivity of a 2D strip

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Submitted 29 August 2014

A strip of the 2D HgTe topological insulator is studied. The same-spin edge states in an ideal system propagate in opposite directions on different sides of the strip and do not mix by tunneling. Impurities, edge irregularities, and phonons produce transitions between the contra-propagating edge states on different edges. This backscattering determines the conductivity of an infinitely long strip. The conductivity at finite temperature is determined in the framework of the kinetic equation. It is found that the conductivity exponentially grows with the strip width. In the same approximation the non-local resistance coefficients of a 4-terminal strip are found.

DOI: 10.7868/S0370274X1421005X

Introduction. Topological insulator (TI) is a novel actively developing field of the solid state physics (see, e.g., reviews [1, 2] and references therein). The main property of TI is topological protection of the edge states that is the spin conservation together with the direction of propagation. As a consequence, the nonlocal transport appears and the conductance at zero temperature is quantized.

The topological protection (TP) is a rigorous consequence of the time reversibility. In mathematical formulation single-electron elastic backscattering processes are forbidden due to conservation of the Z_2 topological index in the systems with an odd number of edges [3, 4, 5], in particular in the case of a single edge. The single-edge states stay robust against not only elastic scattering but against the inelastic phonon scattering [6] both for non-interacting electrons and for Tomonaga-Luttinger liquid. On the contrary, the inclusion of the random Rashba spin-orbit coupling together with the e - e interaction opens the backscattering channel in intraedge e - e scattering [7]. The intraedge e - e backscattering also appears due to k -dependent Rashba interaction [8]. Another variant of non-magnetic intraedge backscattering is two-particle impurity scattering [9]. In macroscopic 2D TI the backscattering appears with participation of electron puddles inside the sample [10, 11]. All these inelastic processes manifest themselves at finite temperature. However, the elastic transitions between contra-propagating states can occur if the system

possesses multiple edges (at least two on different sides of the strip), e.g. in the region of the strip constriction owing to non-adiabatic tunneling [12].

In sufficiently wide strips the elastic interedge backscattering processes are weak. However, they exist due to disorder. There are no papers considering the disorder-induced interedge transitions so far.

The experimental evidence of the edge (and quantized) character of the transport in macroscopic HgTe quantum wells was presented in [13]. The destruction of the quantized conductance by a weak magnetic field shows that these properties are clearly connected with time reversibility. The experiments on the local and non-local conductance of 2D HgTe TI have been recently made [14, 15]. The authors demonstrate that the backscattering length in TI reaches macroscopic values up to 1 mm. At the same time, the authors consider that the violation of the topological protection can be caused by spin-flip processes.

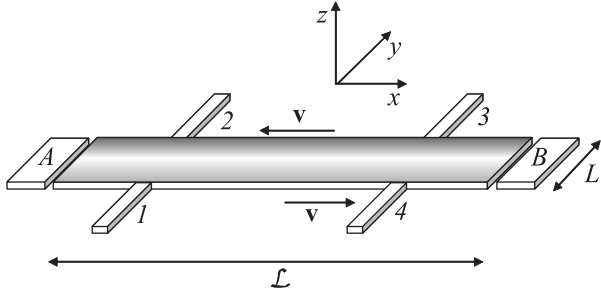
In the present paper we study the free-electron interedge backscattering in a narrow 2D TI strip caused by non-magnetic impurities, edge imperfectness, and phonons and the influence of backscattering on conductivity. The paper is organized as follows. First, we find the electron states in a clean strip. Then, we consider the scattering of edge electrons. Here we will study the problem in the framework of the kinetic equation. The contra-propagating edge states are assumed as the basic states for the kinetic equation. The backscattering mean free time determines the conductivity of the infinitely long system. We examined the backscattering

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mechanisms caused by the impurities, the border imperfectness and phonons. Then we studied the non-local 4-terminal resistance of the TI strip. And after that we discuss the results.

We will neglect the e - e interaction that is justifiable if the e - e interaction constant is small.

Problem formulation. The considered system is a strip of 2D TI from the CdTe/HgTe/CdTe quantum well (see Figure). The strip in the (x, y) plane is determined



Sketch of the TI strip. Edge states are darkened. The directions of velocity \mathbf{v} correspond to $\Sigma_z = 1/2$. (For $\Sigma_z = -1/2$ the directions are opposite.) A and B are the contacts for 2-terminal conductance measurement, 1-4 are contacts for the 4-terminal measurement of non-local conductance

by inequalities $-\mathcal{L}/2 < x < \mathcal{L}/2$, $-L/2 < y < L/2$, $\mathcal{L} \gg L$. We suppose zero boundary conditions on the edges $y = \pm L/2$ and periodic conditions on $x = \pm \mathcal{L}/2$. Our study is based on the effective 2×2 edge-states Hamiltonian $\hat{H}_0 = v\hat{\sigma}_z k_x$, where σ is the Pauli matrix, $\hbar = 1$. This Hamiltonian can be deduced [16] from the initial 2D Hamiltonian for a CdTe/HgTe/CdTe quantum well [17]:

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} H(\mathbf{k}) & 0 \\ 0 & H^*(-\mathbf{k}) \end{pmatrix},$$

$$H(\mathbf{k}) = \epsilon_k + \mathbf{d}\sigma, \quad (1)$$

where $\epsilon_k = -D(k_x^2 + k_y^2)$, $d_x = Ak_x$, $d_y = Ak_y$, $d_z = \mathcal{M}(k) = M - B(k_x^2 + k_y^2)$. Parameters A, B, D, M are determined by the material parameters and the thickness of the quantum well. The upper and lower blocks of the Hamiltonian belong to the Kramers-degenerate states $j_z = 1/2, 3/2$ and $j_z = -1/2, -3/2$ of the 4-fold state $j = 3/2$ of the bulk HgTe zero-momentum point. These blocks can be numerated by the spin quantum number $\Sigma_z = \pm 1/2$ corresponding to the spin Σ degree of freedom. Owing to the Kramers degeneracy it is sufficient to solve the Schrödinger equation for the upper block of Eq. (1) corresponding to $\Sigma_z = 1/2$. In the case of small longitudinal momenta k_x (axis x is chosen along

the strip) and large enough width L one can write for the energy spectrum and wave functions [16]:

$$\Psi_{k_x; \sigma}(x, y) = \frac{e^{ik_x x}}{\sqrt{\mathcal{L}}} \psi_\sigma(y),$$

$$\psi_\sigma(y) = \tilde{c}_\sigma g_\sigma(y) (1, -\sigma\eta), \quad (2)$$

$$g_\sigma(y) = [f_+(y) - \sigma f_-(y)].$$

Here energies $E_\sigma(k_x) = \sigma v k_x$, ($\sigma = \pm 1$) are counted from $E_0 = -MD/B$, $v = A\sqrt{B_+ B_-}/B^2$, $B_\pm = B \pm D$, \tilde{c}_σ are the normalization constants. The expressions for $f_\pm(y)$ are given by Eqs. (7), (8) in [16].

In the limit of large L and small k_x expressions for functions $g_\sigma(y)$ are simplified and given by:

$$g_\sigma(y) \simeq 2[e^{-\lambda_1 L/2 - \sigma \lambda_1 y} - e^{-\lambda_2 L/2 - \sigma \lambda_2 y}]. \quad (3)$$

The quantity σ is conserved in a clean system and one can consider $\sigma/2$ as a pseudospin. Functions $\psi_\sigma(y)$ exponentially decay from the edges $y = -\sigma L/2$, correspondingly. Functions with different σ are weakly overlapped with each other if $\lambda_{1,2} L \gg 1$. In fact, the wave functions given by Eqs. (2), (3) correspond to insulated edges. This approximation is valid for a sufficiently large electron energy exceeding the gap Δ [16]:

$$|E| \gg \Delta = 4 \frac{|AB_+ B_- M|}{\sqrt{B^3(A^2 B - 4B_+ B_- M)}} e^{-\lambda_2 L}.$$

Due to the exponential decay of Δ with increase of L this limitation can be easily fulfilled.

The presence of disorder (impurities, edge roughness, phonons) leads to the transitions between edge states with different σ . Decay rate λ_1 is larger than λ_2 . In the limit of a large L this permits to keep only one exponent with λ_2 in $g_\sigma(y)$ when one calculates overlapping integrals.

In the same approximation for η , \tilde{c}_σ , and $\lambda_{1,2}$ we have

$$\eta^2 = \frac{B_+}{B_-}, \quad \tilde{c}_{+1}^2 \simeq \tilde{c}_{-1}^2 \equiv \tilde{c}^2 = \frac{AMB_- \sqrt{B_+ B_-}}{4B(A^2 B - 4MB_+ B_-)}, \quad (4)$$

$$\lambda_{1,2} = \frac{A}{2\sqrt{B_+ B_-}} \pm \sqrt{\frac{A^2}{4B_+ B_-} - \frac{M}{B}}, \quad (5)$$

$$\lambda_1 + \lambda_2 = \frac{A}{\sqrt{B_+ B_-}}, \quad \lambda_1 \lambda_2 = \frac{M}{B}.$$

The basic Hamiltonian results from the 2D Hamiltonian (1) when $\lambda_{1,2} \gg k_x, 1/L$. It should be complemented by the potential of interaction with defects. In the same representation the potential is given by the 2×2 matrix $\hat{U}(x)$ with matrix elements being equal to

$U_{\sigma'\sigma}(x) = \langle \psi_{\sigma'}(y) | U(x, y) | \psi_{\sigma}(y) \rangle$ which are composed by a projection of the potential to the states $\psi_{\sigma}(y)$. This matrix depends on coordinate x only. The total edge-state Hamiltonian reads

$$\hat{H} = -iv\hat{\sigma}_z\partial_x + \hat{U}(x). \quad (6)$$

Impurity scattering. In the kinetic approach the conductivity is caused by the transitions of electrons between the edge states. In this section we will find the transition probability under scattering on the impurities located inside the strip. The potential energy of interaction of an electron with impurities is given by

$$U_{\text{imp}} = \sum_n u_n(\mathbf{r}) = \sum_n u(\mathbf{r} - \mathbf{r}_n) = \sum_{\mathbf{q}, n} \tilde{u}_{\mathbf{q}} e^{i\mathbf{q}(\mathbf{r} - \mathbf{r}_n)}, \quad (7)$$

where $\tilde{u}_{\mathbf{q}} = \int u(\mathbf{r}) e^{-i\mathbf{q}\mathbf{r}} d\mathbf{r} / S$ is the Fourier transform of the potential of an individual center, $S = L\mathcal{L}$ is the area of the system.

We will be interested in transitions with backscattering. The necessary matrix elements of corresponding matrix $\hat{U}(x)$ can be written as

$$U_{+1;-1}(x) = U_{-1;+1}(x) = \tilde{c}^2(1 - \eta^2) \times \\ \times \sum_{\mathbf{q}, n} \tilde{u}_{\mathbf{q}} e^{iq_x(x-x_n) - iq_y y_n} \int_{-L/2}^{L/2} dy g_{+1}(y) g_{-1}(y) e^{iq_y y}. \quad (8)$$

Again, in case of a large L one can find an approximate expression for $\int dy g_{+1}(y) g_{-1}(y) e^{iq_y y}$ at $\lambda_1 > \lambda_2$:

$$\int dy g_{+1}(y) g_{-1}(y) e^{iq_y y} \simeq \delta_{q_y, 0} \cdot 4L e^{-\lambda_2 L}. \quad (9)$$

As a result for the electron interaction with an individual impurity, we have

$$u_{\sigma; -\sigma}(x) = 4L e^{-\lambda_2 L} \tilde{c}^2(1 - \eta^2) \sum_{q_x} \tilde{u}_{q_x, 0} e^{iq_x x}. \quad (10)$$

Using Eq. (10) we can write the transition probability between states $|k'_x; \sigma\rangle$ and $|k'_x; -\sigma\rangle$ as follows:

$$W_{k'_x, -\sigma; k_x, \sigma}^{(\text{imp})} = \\ = 32\pi N \tilde{c}^4 (1 - \eta^2)^2 |\tilde{u}_{2k_x, 0}|^2 L^2 e^{-2\lambda_2 L} \delta[v(k'_x + k_x)], \quad (11)$$

where N is the total number of scattering centers. In Eq. (11) averaging over distribution of impurities have been carried out. Eq. (11) can be presented in the form:

$$W_{k'_x, -\sigma; k_x, \sigma}^{(\text{imp})} = \frac{\pi}{\mathcal{L}\tau} \delta(k'_x + k_x), \quad (12)$$

where we have introduced the relaxation time due to impurity scattering:

$$\frac{1}{\tau} = \frac{8n_s}{v} |\tilde{u}_{2k_x, 0}|^2 L e^{-2\lambda_2 L} \lambda_2^2 a, \\ a = \left[\frac{1 - \eta^2}{1 + \eta^2} \frac{\lambda_1(\lambda_1 + \lambda_2)}{(\lambda_1 - \lambda_2)^2} \right]^2.$$

Here $\tilde{u}_{\mathbf{q}} = \tilde{v}_{\mathbf{q}} / (L\mathcal{L})$, $n_s = N/S$ is the impurity concentration.

Scattering on edge imperfections. Let the edges be imperfect, namely having shapes $y = \sigma L/2 + h_{\sigma}(x)$, where $h_{\sigma}(x)$ are random functions with correlators $\langle h_{\sigma}(x) h_{\sigma'}(x') \rangle = w_{\sigma} \delta(x - x') \delta_{\sigma, \sigma'}$. Electron interaction with roughness of edges is determined by the pseudo-potential [18, 19]:

$$U_{\text{edge}} = \frac{1}{2m} \sum_{\sigma} h_{\sigma}(x) \hat{k}_y \delta(y + \sigma L/2) \hat{k}_y. \quad (13)$$

On the analogy with the impurity case we obtain for the transition probability caused by the edge imperfectness Eq. (12) with replacement of the relaxation time by

$$\frac{1}{\tau} = \frac{8}{m^2 v} (w_{+1} + w_{-1}) e^{-2\lambda_2 L} \lambda_2^4 (\lambda_1 - \lambda_2)^2 a. \quad (14)$$

The order of w_{σ} is determined by the typical height h_0 and width w_0 of roughness: $w_{\sigma} \sim h_0^2 w_0$.

Conductivity. Let us consider a long strip in a longitudinal external electric field \mathcal{E} . The linearized kinetic equation for the edge state electrons is:

$$\sigma e \mathcal{E} v \frac{\partial f_0[E_{\sigma}(k_x)]}{\partial E} = \sum_{k'_x} W_{k'_x, -\sigma; k_x, \sigma} (\chi_{\sigma, k'_x} - \chi_{\sigma, k_x}). \quad (15)$$

Here $f_{\sigma, k_x} = f_0[E_{\sigma}(k_x)] + \chi_{\sigma, k_x}$ is the distribution function, $f_0[E_{\sigma}(k_x)]$ is the Fermi function. Eq. (15) is easily solved using identity $\chi_{-\sigma, -k_x} = -\chi_{\sigma, k_x}$:

$$\chi_{\sigma, k_x} = -\sigma e \mathcal{E} \frac{\partial f_0[E_{\sigma}(k_x)]}{\partial E} v \tau, \quad (16)$$

where τ is the relaxation time. For $1/\tau$ one should utilize the sum of scattering rates due to all considered mechanisms. As a result, we obtain the classical conductivity of degenerate electron gas $G_0 l$ and the corresponding conductance of a finite strip $G_0 l / \mathcal{L}$ expressed via the conductance quantum $G_0 = 2e^2/h$ and the mean free path $l = v\tau$ at the Fermi energy.

Phonon mechanisms of electron backscattering. The impurity scattering conserves the phase coherence and hence, strictly speaking, cannot be considered within the kinetic equation approach. However, this is not the case when any decoherence factor is taken into account. A sufficiently strong decoherence revives the kinetic equation's applicability. Below we consider the backscattering of electrons by phonons. Note, that at high enough temperature, the phonon backscattering can be considered in the same way as the impurity scattering neglecting the emitted phonon frequency

as compared to the temperature. The Hamiltonian of electron-phonon interaction is

$$H_{e-ph} = \sum_{k,\sigma,k'\sigma',\mathbf{q}} c_{\mathbf{q}} J_{q_z} J_{q_y;\sigma'\sigma} a_{\sigma',k'}^+ a_{\sigma,k} b_{\mathbf{q}}^+ \delta_{k'-k,q_x} + \text{h.c.} \quad (17)$$

Here $a_{\sigma,k}^+$, $a_{\sigma,k}$ are the edge electron creation/annihilation operators, $b_{\mathbf{q}}^+$, $b_{\mathbf{q}}$ are the creation/annihilation operators of bulk longitudinal acoustic phonons with 3D momentum \mathbf{q} , $c_{\mathbf{q}} = \Lambda q / \sqrt{2\rho\omega_{\mathbf{q}}\Omega}$, $J_{q_y;\sigma'\sigma} = \langle \sigma' | e^{iq_y y} | \sigma \rangle$, $J_{q_z} = \int dz \zeta^2(z)$, where Λ is the deformation potential constant, ρ is the crystal density, Ω is the system volume, $\omega_{\mathbf{q}} = cq$ is the phonon frequency (c being the sound velocity), $\zeta(z)$ is the ground state wave-function of the quantum well CdTe/HgTe/CdTe. In our consideration it is assumed that electrons interact by the deformation potential with the bulk longitudinal acoustic phonons only; the difference between HgTe and CdTe elastic constants and deformation potentials is neglected.

Similar to Eq. (11), we have found the interedge ($\sigma \rightarrow -\sigma$) transition probability caused by the phonons. As a result, instead of Eq. (11), we have for the backscattering time

$$\frac{1}{\tau} = \frac{8\Lambda^2 L T \lambda_2^2 e^{-2\lambda_2 L}}{v\rho c^2} a \int \zeta^4(z) dz. \quad (18)$$

The integral in Eq. (18) has the order of the inverse quantum well width $1/d$. (It should be noted that, in contrast to the impurity scattering, the scattering due to phonons requires accounting for the transversal (i.e. along z) structure of the edge state.) In deducing Eq. (18), we have utilized the condition that temperature T is much higher than the characteristic frequency of emitted phonons c/d . The phonon-induced backscattering grows with the temperature and has the same smallness caused by the overlapping of edge states as the impurity scattering. Note, that the electron-phonon scattering rate Eq. (18) can be found by replacement of the total impurities number by the phonon distribution function and the corresponding replacement of the interaction constant. For conductivity one should collect the relaxation rates caused by impurities, edges and phonons together.

Now go to the forward phonon-induced scattering $\sigma \rightarrow \sigma$. This process, being essentially stronger than the backscattering, conserves the electron velocity and, hence, does not affect the kinetics. The role of the forward scattering is to control the phase coherence in the system, namely electron dephasing time τ_{ϕ} .

The validity of the kinetic regime needs $\tau_{\phi}(T) \ll \tau$, *vice versa* the localization occurs if $\tau_{\phi}(T) \gg \tau$; the transition between these regimes occurs when $\tau_{\phi}(T) \sim \tau$,

where τ in the low-temperature limit does not depend on T . A more detailed consideration goes beyond the scope of this paper.

Discussion. In conclusion, we have found the conductivity of the infinitely long strip of the 2D TI. At finite temperature the kinetic equation approach is valid. In this approximation the conductivity is determined by the mean free path due to the interedge backscattering on impurities, edge imperfections and phonons. The non-local 4-terminal resistance coefficients have been also found. The validity of the kinetic-equation approach is limited by the dephasing caused by the phonon-induced intraedge scattering. At low enough temperatures the kinetic-equation approach becomes invalid and should be replaced by the consideration based on the localization of electrons; this situation and the dephasing mechanism at higher temperature will be studied later on.

Thus, we demonstrated that a long TI strip like 1D wire of usual conductor possesses the finite conductivity at high temperatures in presence of the interedge scattering. The difference with a quantum wire consists in exponentially long (with respect to the strip width) mean free path.

Let us discuss the correspondence with the experimental measurements [14, 15]. In experiments [14, 15] it was found that the conductivity of a macroscopic 2D TI is: i) non-local, ii) non-quantized, and iii) temperature-independent at low temperature. Feature i) means the edge character of conductivity while, ii) means deflection from the ballistic transport due to the backscattering. Feature iii) indicates the impurity mechanism of the backscattering. Very large macroscopic backscattering length in [14] suggests a weak influence of spin-flip scattering. The macroscopic system in [14, 15] is not the narrow strip considered here. In a macroscopically wide device the transitions between the strip edge are forbidden. However, we think that the real TI can have many puddles of a normal semiconductor phase due to the fluctuations of the HgTe quantum well thickness. These puddles provide the existence of multiple inner edges between TI and a normal semiconductor. The chain of transitions between these edge states shall produce a transition to the other external edge with the opposite direction of motion. If the impurities (edge imperfections) give the main contribution to this process in conditions of destroyed coherence, one may expect no temperature dependence of the conductivity in accordance with [14, 15]. This possibility is alternative to the process discussed in [10, 11].

It should be emphasized that our consideration is limited by the case when the electron energy exceeds

the gap caused by interaction between edges. This limitation is not critical due to the exponentially small gap value. Note also, that we have neglected the spin non-conservation caused by the spin-orbit interaction, magnetic impurities, and superfine interaction. These mechanisms go beyond the paper's scope, but look weaker than considered ones.

The work was supported by the RFBR grants # 13-0212148 and 14-02-00593.

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