Helical edge transport in the presence of a magnetic impurity

P. D. Kurilovich$^{1,2,3}$, V. D. Kurilovich$^{1,2,3}$, I. S. Burmistrov$^{4,1,4,51}$, M. Goldstein$^6$

$^1$ Moscow Institute of Physics and Technology, 141700 Moscow, Russia
$^2$ Skolkovo Institute of Science and Technology, 143026 Moscow, Russia
$^3$ L. D. Landau Institute for Theoretical Physics RAS, 119334 Moscow, Russia
$^4$ Institut für Theorie der kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany
$^5$ Institut für Nanotechnologie, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany
$^6$ Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, Tel Aviv 6997801, Israel

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We consider the effects of electron scattering off a quantum magnetic impurity on the current-voltage characteristics of the helical edge of a two-dimensional topological insulator. We compute the backscattering contribution to the current along the edge for a general form of the exchange interaction matrix and arbitrary value of the magnetic impurity spin. We find that the differential conductance may exhibit a non-monotonous dependence on the voltage with several extrema.

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Introduction. — Two-dimensional topological insulators (2D TIs) are in the focus of recent interest due to existence of two helical edge states inside the band gap $[1,2]$. Because of spin-momentum locking caused by strong spin-orbit coupling, electrical current transfers helicity along the edge $[3,4]$. This “spin” current is a hallmark of the quantum spin Hall effect, and it has been detected experimentally in HgTe/CdTe quantum wells $[5,9]$. If only elastic scattering is allowed, and in the absence of time-reversal symmetry breaking, the helical state is a realization of the ideal transport channel $[3,4]$. This prediction was questioned by the experiments in HgTe/CdTe $[5,10–12]$.

For the sake of simplicity, we neglect quadratic terms and consider simplified version, $[15,16]$ or $S \geq 1/2$ $[27,28]$. In this Letter we study theoretically a modification of the ideal current-voltage characteristics of the helical edge in 2D TI by weak scattering off a single magnetic impurity. As a physical realization of such system we have in mind the (001) CdTe/HgTe/CdTe quantum well (QW) with a Mn impurity that possesses spin $S = 5/2$. Contrary to the previous works, we consider a general structure of the matrix describing exchange interaction between edge states and magnetic impurity $[cf. \ Eq. (6)]$. For $S = 1/2$ we find an analytical expression for the backscattering current at arbitrary voltage. For larger spin, $S > 1/2$, we obtained analytical expressions for the backscattering current at low and high voltages.

Model. — The low-energy physics of electron and hole states in 2D TI based on the (001) CdTe/HgTe/CdTe quantum well (QW) is described by Bernevig-Hughes-Zhang (BHZ) Hamiltonian $[3]$. This Hamiltonian is a $4 \times 4$ matrix in the basis of electron and heavy-hole states $|E_1, +\rangle$, $|H_1, +\rangle$, $|E_1, -\rangle$, $|H_1, -\rangle$, with elements which are linear and quadratic functions of the momentum $k = \{k_x, k_y\}$. For the sake of simplicity, we neglect quadratic terms and consider simplified version,

$$H = \begin{pmatrix}
h(k) & 0 \\
0 & h^T(-k)
\end{pmatrix}, \quad h(k) = \begin{pmatrix}
M & Ak_+ \\
Ak_- & -M
\end{pmatrix}, \quad (1)$$

where $A$ and $M$ are material parameters which depend on the thickness of the QW, $k_\pm = k_x \pm ik_y$, and the su-

1) e-mail: burmi@itp.ac.ru.
In order to describe the appearance of the edge states in the presence of boundary situated at \( x = 0 \), we adopt the approach by Volkov and Pankratov [29]. We assume that inside the 2D TI \((x < 0)\) the mass \( M \) in the Hamiltonian \([1]\) is negative, whereas outside \((x > 0)\) the mass is equal to \(+\infty\). Then, as shown in Ref. [29], a pair of edge states appears as the solution of the Schrödinger equation with the Hamiltonian \( H(−i\partial_x, k_y) \). These edge states are connected by time-reversal symmetry, and for a given \( k_y \) have the following form:

\[
\psi_{\text{edge},+}(k_y, r) = (1\ i\ 0\ 0)^T e^{i k_y y} e^{-|x|/\xi} \theta(-x),
\]

\[
\psi_{\text{edge},-}(k_y, r) = (0\ 0\ 1\ −i)^T e^{i k_y y} e^{-|x|/\xi} \theta(-x),
\]

where \( \xi = A/|M| \) denotes the characteristic width of the edge states, and \( \theta(x) \) stands for the Heaviside step function. The effective 2 \( \times \) 2 Hamiltonian for the edge states can be obtained by projection of the 4 \( \times \) 4 Hamiltonian \([1]\) onto the edge states subspace \([2]\):

\[
H^{(0)}_{\text{edge}} = -A k_y \sigma_z.
\]

The Pauli matrices \( \sigma_x, \sigma_y, \) and \( \sigma_z \) operate in the basis of edge states. The Hamiltonian \([3]\) gives rise to linear dispersion, \( \epsilon_{1/2}^{(\text{edge})}(k_y) = \mp A k_y \).

After the projection onto the subspace of 2D electron and hole states \(|E_1, +\rangle, |H_1, +\rangle, |E_1, -\rangle, |H_1, -\rangle\), the Hamiltonian of a magnetic impurity with spin \( S \) situated at some point \(|x_0, y_0, z_0\rangle\) within the (001) quantum well can be written as follows \([28,30]\):

\[
H_{\text{imp}} = J_{\text{bulk}} \delta(x-x_0) \delta(y-y_0),
\]

where the matrix \( J_{\text{bulk}} \) reads \((S_z = S)\) and \( J_{\text{bulk}} \) reads \((S_z = S-1\), \( S_z = 2 \), respectively, and \( J_{\text{bulk}} \) reads \((S_z = 2, S_z = -1)\), that do not conserve the \( z \) component of the effective angular momentum. These transitions are allowed because the edge states \([2]\) are superpositions of \(|E_1, \pm\rangle\) states with \( z \) component of the angular momentum being equal to \( \pm 1/2 \), respectively, and \(|H_1, \pm\rangle\) states for which this component equals \( \pm 3/2 \).

We mention that the Hamiltonian \([1]\) does not take into account a possible reduction of the rotational symmetry in the \( x-y \) plane. Time-reversal symmetry allows for non-zero off-diagonal terms in the bulk Hamiltonian due to the presence of bulk \([32,35]\) or interface \([30,37]\) inversion asymmetry. These off-diagonal terms result in a splitting of the electron and heavy-hole states, which has been measured recently in CdTe/HgTe/CdTe \([38,39]\). Furthermore, the presence of the off-diagonal terms leads to a modification of the edge states \([33,37]\) and, consequently, the matrix \( J \) acquires a general form with no vanishing elements \([40]\).

**One-loop renormalization.** — The Hamiltonian \([40]\) is a typical Hamiltonian for an anisotropic Kondo problem (see Ref. [41] for a review). It was derived at the energy scale of the order of the bulk gap \(|M|\). Since below we are interested in edge transport which occurs at energy scales \( \max\{|T, |V|\} \ll |M| \), we need to take into account the renormalization of the exchange Hamiltonian \([6]\).
The interaction between the edge electrons and the magnetic impurity modifies the structure of the interaction matrix $J$, leading to the Kondo effect at low temperatures. We assume that the exchange interaction is weak, $|J_{jk}| \ll 1$. Then renormalization of the exchange matrix $J$ can be described within the one-loop renormalization group (RG) equations. For a general form of the matrix $J$ and arbitrary spin they become [41]

$$
\frac{dJ_{jk}}{dl} = \frac{1}{2} \varepsilon_{zmns} \varepsilon_{kps} J_{np} J_{ms}.
$$

Here $l = \ln(|M|/E)$ is the running RG logarithmic scale and $\varepsilon_{zmns}$ stands for the Levi-Civita symbol. The band gap $|M|$ serves as the ultraviolet cutoff whereas $E = \max(T, |V|)$ determines the infrared energy scale. Using Eqs. (8), one can find the following equations,

$$
\frac{d(JJ^T)_{jk}}{dl} = \frac{d(J^TJ)_{jk}}{dl} = 2 \delta_{jk} \det J.
$$

It is convenient to perform the singular value decomposition of the initial matrix, $J(l = 0) = R \Lambda R^T$, where the $SO(3)$ matrices $R_{<,>}$ do not flow, and where $\Lambda = \text{diag}(\lambda_1, \lambda_2, \lambda_3)$. Then, in the course of the RG flow, the matrix $\Lambda$ preserves its diagonal form with $\lambda_j$ satisfying the following equations

$$
\frac{d\lambda_1}{dl} = \lambda_2 \lambda_3, \quad \frac{d\lambda_2}{dl} = \lambda_1 \lambda_3, \quad \frac{d\lambda_3}{dl} = \lambda_1 \lambda_2.
$$

Eqs. (10) have the two independent invariants $\lambda_1^2 - \lambda_2^2$ and $\lambda_2^2 - \lambda_3^2$. In the general case, if none of these invariants is zero, the RG flow tends to the manifold $|\lambda_1| = |\lambda_2| = |\lambda_3|$ with $\lambda_1 \lambda_2 \lambda_3 > 0$. All three $\lambda_j$ diverge at a finite scale $l_K$, which determines the Kondo temperature $T_K = |M|e^{-1/\lambda_1}$. In what follows, we assume that $\max(T, |V|) > T_K$ so that $|J_{jk}| \ll 1$ at the corresponding scale.

**Backscattering current and master equation.** — In order to obtain the correction to the current flowing along the edge due to scattering off a magnetic impurity, we shall follow an approach developed recently in Ref. [26]. The helicity of the edge states allows one to relate the correction to the current, $\Delta I$, to the rate of change of the $z$ component of the total spin of the edge electrons:

$$
\Delta I = \left\langle \frac{d}{dl} \int dy \left( s_z \right) \right\rangle, \quad s_z(y) = \frac{1}{2} \Psi^\dagger(y) \sigma_z \Psi(y),
$$

where $\Psi^\dagger$ and $\Psi$ denote creation and annihilation operators of the edge electrons, respectively.

The $z$ component of the total spin of the edge electrons is not conserved due to the exchange interaction with the magnetic impurity, Eq. (9). To second order in the exchange interaction $J_{jk}$ we find [40],

$$
\frac{\Delta I}{G_0 V} = \frac{\pi^2}{2} \left[ \langle \chi y \rangle \langle s_z \rangle \coth \frac{V}{2T} - 2 \sum_{k=x,y} \langle J_{mk} J_{pk} \rangle \langle S_m S_p \rangle \right].
$$

(12)

Here $\chi y = 2 \varepsilon_{jkli} J_{kl} J_{yi}$ and $\langle \cdots \rangle$ denotes the average with respect to the steady-state reduced density matrix $\rho_S$ of the impurity spin, e.g., $\langle S_y \rangle = Tr S_y \rho_S$. In order to determine the steady state we derived the following equation for the density matrix of the impurity spin within second order perturbation theory in $J_{jk}$ [40],

$$
\frac{d\rho_S}{dl} = \frac{(s_z)_{jk} J_{jk}}{IV} [S_j, \rho_S] + \eta_{jk} \left( S_j \rho_S S_k - \frac{1}{2} \{ \rho_S, S_l S_j \} \right).
$$

(13)

Here the average $z$ component of the edge spin density $\langle s_z \rangle = \nu V/2$ is evaluated disregarding the influence of the impurity on the distribution of the edge electrons. The matrix $\eta$ is defined as $\eta = \pi T J J^T / 2$, where

$$
\Pi_V = \begin{pmatrix} V/2 & \coth V/2 & -iV/2 & 0 \\ iV/2 & 0 & V/2 \coth V/2 & 0 \\ -iV/2 & V/2 \coth V/2 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.
$$

(14)

We note that the eigenvalues of $\Pi_V$ are equal to 1 and $(V/2T)\coth(V/2T) \pm 1 \geq 0$. Therefore, the matrix $\eta$ is positive semidefinite and the master equation (13) has the Lindblad form, ensuring the positivity of $\rho_S$ [42].

The vector $\langle s_z J_{jk} \rangle$ plays the role of the effective magnetic field in which the impurity spin rotates, whereas $\eta_{jk}$ is responsible for Korringa-type relaxation.

The expression for the correction to the current [12] and the master equation [13] are invariant under rotation of the exchange matrix $J$ from the left by an arbitrary orthogonal matrix $U$, $J \rightarrow UJ$. Indeed, since the following relation holds, det $J = \chi y J_{jk}/2$, the vector $X$ transforms as follows: $X \rightarrow UX$.

Using the steady state solution of the Lindblad equation [13] one can compute the averages in Eq. (12) and find $\Delta I$. For example, multiplying both sides of Eq. (13) by $S_q$ and taking the trace, we derive the following equation for the average impurity spin:

$$
\frac{d\langle S_q \rangle}{dt} = \frac{\pi T}{2} \left[ \frac{V}{2T} \varepsilon_{xkl}\varepsilon_{yqr} J_{mk} J_{pl} \langle \{ S_r, S_p \} \rangle - \Gamma_{qr} \langle S_r \rangle \right],
$$

(15)

where we introduced the following $3 \times 3$ matrix

$$
\Gamma_{qr} = \frac{1}{\pi T} \left[ \delta_{qr} \text{Tr} \eta - \frac{\eta_{yq} + \eta_{rq}}{2} + V \varepsilon_{yqr} J_{yz} \right].
$$

(16)

In general it is not an easy task to find the averages analytically, since $\langle S_r \rangle$ is related to $\langle \{ S_m, S_p \} \rangle$, etc.
Linear conductance. — In spite of the complicated structure of the master equation \([13]\) for an arbitrary value of the impurity spin \(S\), the correction to the linear conductance, \(\Delta G = \lim_{V \to 0} \Delta I/V\), can be found analytically. As one can see from Eq. \([12]\), it is enough to compute \(\langle \{S_r, S_p\} \rangle\) for \(V = 0\), and to find \(\langle S_r \rangle\) to the first order in \(V\). Using the fact that at zero bias voltage \(\langle \{S_r, S_p\} \rangle = 2 S(S+1)\delta_{rp}/3\), we find from Eq. \([15]\):

\[
\langle S_r \rangle = \frac{S(S+1)V}{T} (\Gamma_0^{-1})_{rq} \chi_q.
\]

Here we introduce \(\Gamma_0 = \text{Tr}(\mathcal{J} \mathcal{J}^T - \mathcal{J}^T \mathcal{J})\), which is the matrix \(\Gamma\) evaluated at \(V = 0\). Then, from Eq. \([12]\) we obtain the following correction to the conductance

\[
\frac{\Delta G}{G_0} = \frac{\pi^2 S(S+1)}{3} \left[ \chi^T \Gamma_0^{-1} \chi - g \right],
\]

where \(g = (\mathcal{J}^T \mathcal{J})_{xx} + (\mathcal{J} \mathcal{J}^T)_{yy}\). Interestingly, the impurity spin enters \(\Delta G\) as an overall factor \(S(S+1)\) only.

For a spin \(S = 1/2\) the correction \(\Delta G/G_0\) is exactly zero \([16]\). Therefore, the correction is zero for any exchange matrix of the form \(U \mathcal{J}^{(iso)}\). If one neglects the renormalization of the effective magnetic field mediated by the interaction with the electrons, then one can plug Eq. \([7]\) into Eq. \([19]\) to find

\[
\Delta G = -\frac{4S(S+1)M^2 J_0 J_m^2 e^{-4|\alpha|/\xi}}{3} \frac{A^2}{J_m^2 + J_2^2 + 2J_0^2}.
\]

Backscattering current for spin \(S = 1/2\). — In the case of a spin \(S = 1/2\) impurity we can find the backscattering current at arbitrary values of \(V\). Since \(\langle S_r, S_p \rangle = \delta_{rp}/2\) for spin \(S = 1/2\), Eq. \([13]\) leads to the stationary solution \(\langle S_r \rangle = V(\Gamma_0^{-1})_{rq} \chi_q/(4T)\). Simultaneously, the correction to the current, Eq. \([12]\), is expressed via \(\langle S_r \rangle\) only. Finally, we find

\[
\Delta I = G_0 \frac{\pi^2 V}{4} \left[ X^T \Gamma_0^{-1} X \frac{V}{2T} \coth \frac{V}{2T} - g \right].
\]

For an exchange matrix of the form \(U \mathcal{J}^{(iso)}\) the backscattering correction to the current is zero at any voltage \([16]\).

Backscattering current for an arbitrary spin. — In the case of spin \(S > 1/2\) the master equation \([13]\) cannot be reduced to a closed equation for the average spin. However, at large voltage, \(|V| \gg \max(\{|J_{jk}|\})\), one can find the stationary solution of the master equation \([13]\) in the following way. In this regime the first term in the right hand side of Eq. \([13]\) dominates over the second one. Let us introduce the effective Hamiltonian \(H_V = -\langle s_z \rangle J_z S_j / \nu\). Then, it is reasonable to look for a stationary density matrix which commutes with \(H_V\), i.e., which is diagonal in eigenbasis of \(H_V\). The right hand side of the Lindblad equation \([13]\) then yields

\[
\rho_{S,m} = \frac{\eta_{jk} \langle |S_j| m \rangle \rho_{S,m} \langle m | S_k \rangle}{\eta_{jk} \langle |S_k| j \rangle}. \tag{23}
\]

Here \(|l|\) and \(|m\) denotes eigenstates of \(H_V\), i.e. states with a given angular momentum projection in the direction of the effective magnetic field mediated by the interaction with the electrons, while \(\rho_{S,m} = \langle m | \rho S | m \rangle\). Since the Hamiltonian \(H_V\) is linear in the spin operators, its eigenenergies are linear functions of \(l\). Furthermore, the intermediate states \(m\) in Eq. \([23]\) are equal to \(l\) or \(l \pm 1\) only. Hence, it is possible to solve Eq. \([23]\) by the Gibbs ansatz \([10]\):

\[
\rho_{S,m} = \exp(-H_V/T_{eff}) / \text{Tr} \exp(-H_V/T_{eff}).
\]

Then, upon summation over \(l\), Eq. \([23]\) becomes equivalent to the following equation:

\[
\eta_{jk} \text{Tr} \left( S_k S_j \right) = \eta_{jk} \text{Tr} \left( e^{H_V/T_{eff}} S_j e^{-H_V/T_{eff}} S_k \right). \tag{24}
\]

In order to find the effective temperature \(T_{eff}\), it is convenient to define the matrix \(C_{jk} = i \varepsilon_{jk} \langle s_z \rangle J_z / \nu\). Then Eq. \([24]\) can be equivalently rewritten as

\[
T_{eff} = \frac{\text{Tr}_\nu \mathcal{C} \text{Tr}_\eta \left[ \mathcal{J} \Gamma_0 \mathcal{J}^T \right]}{\text{Tr}_\nu \mathcal{C} \text{Tr}_\eta \mathcal{J} \Gamma_0 \mathcal{J}^T},
\]

where \(\mathcal{E}_V = \text{diag}(1, 0, -1) V \sqrt{\langle \mathcal{J} \mathcal{J}^T \rangle_{zz}} / 2\) and \(\mathcal{C} = \mathcal{R} \mathcal{E}_V \mathcal{R}^{-1}\). The effective temperature reads

\[
T_{eff} = \frac{V}{4} \sqrt{\langle \mathcal{J} \mathcal{J}^T \rangle_{zz}} \left[ \frac{\arccosh(\langle \mathcal{J} \mathcal{J}^T \rangle_{zz}) \coth \frac{V}{2T}}{2(\det \mathcal{J}) \sqrt{\langle \mathcal{J}^T \mathcal{J} \rangle_{zz}}} \right]^{-1}. \tag{25}
\]
$J$, and is of order $|J_{jk}| \max\{T/|V|\}$. Interestingly, the effective temperature is independent of the value of the spin $S$. Moreover, the Gibbs factor $\exp(-\mathcal{H}_V/T_{\text{eff}})$ is independent of the voltage at $|V| \gg T$. Therefore, at $|V| \gg T$ the impurity spin is not fully polarized. We note that the result in Eq. (25) can be easily expressed via the matrix $R_s$ and parameters $\lambda_j$.

If one neglects the renormalization of $J_{jk}$, then for $J_{jk}$ given by Eq. (1) the effective temperature acquires the following simple form ($J = \sqrt{4J_{0}^2 + J_{z}^2}$):

$$T_{\text{eff}} = \frac{V}{\sqrt{2\, J\,J_{z}}} \left\{ \frac{\text{arccoth} \left[ \frac{J^2 + J_{z}^2}{2JJ_{z}} \coth \frac{V}{2T} \right]}{4\pi \lambda^2} \right\}^{-1}.$$  

(26)

We note that our result (26) is different from the result in Ref. [25], in which the stationary density matrix was determined in the case of the exchange matrix $\gamma$ at $|V| \gg \max\{|J_{jk}| T\}$. The solution obtained in Ref. [28] leads to the full polarization of the impurity spin at $|V| \gg T$. This conclusion is a consequence of the assumption made in Ref. [25] that $\rho_S$ is diagonal in the eigenbasis of $S_z$ rather than $\mathcal{H}_V$, an assumption which is not justified in general.

Having found the effective temperature, one can use the stationary Gibbs-like density matrix to compute the averages $\langle S_r \rangle$ and $\langle S_m S_p \rangle$ appearing in Eq. (12). In this way, one can determine the correction to the current in the regime of large voltage, $|V| \gg \max\{|J_{jk}| T\}$. For spin $S = 1/2$ we reproduce the result (22) in this regime.

An example of the dependence of the backscattering correction to the differential conductance $\Delta G(V)$ on the voltage for the different values of the impurity spin $S$ is shown in Fig. 4. The curves are obtained by numerical solution of the master equation (13) without taking into account the renormalization of $J_{jk}$. For $S > 1/2$ the differential conductance is non-monotonous, with extrema at $V \sim |J_{jk}| T$ and $V \sim T$ (indicated by triangles in Fig. 1). The first extremum is the consequence of competition between the effective magnetic field acting on the impurity spin and the relaxation (the first and second terms in the right hand side of Eq. (13), respectively). The extremum at $V \sim T$ is the consequence of the dependence of the effective temperature on the voltage. In contrast with the higher spins, for $S = 1/2$ the differential conductance saturates already at $V \sim |J_{jk}| T$ instead of $V \sim T$. This feature follows directly from the analytical solution (12). Finally, we mention that in the case of $|V| \ll |J_{jk}| T$ the ratio $\Delta G(V)/\Delta G(0)$ is independent of $S$.

Conclusions. — In conclusion, we presented the results of a detailed study of the backscattering current at a helical edge due to weak scattering off a single Kondo-type magnetic impurity. Contrary to the previous studies we considered the case of a magnetic impurity with an arbitrary spin $S$ and a general exchange matrix. For $S = 1/2$ we found an analytical expression (18) for the backscattering current valid at arbitrary voltage. For spin $S > 1/2$ we found analytical expressions for the backscattering current at low and high voltages.

For a (001) CdTe/HgTe/CdTe QW with width close to the critical one, 6.3 nm, the exchange couplings $|J_m|, |J_z|, |J_0|$ for a Mn impurity can be estimated to be of the order of 0.1 eV nm$^{-2}$ [30]. Using the estimates $\nu \approx 0.5$ eV$^{-1}$ nm$^{-1}$ and $\xi \approx 40$ nm [1], we find that the exchange couplings $J_{jk}$ are of the order $10^{-3}$. This implies that the backscattering correction to the conductance due to a single Mn impurity is of order $-\Delta G/G_0 \sim 10^{-4} \div 10^{-3}$.

Finally, we mention that in the case $S > 1/2$ a local anisotropy term for the impurity spin is generated [43,44], e.g., due to indirect exchange interaction mediated by the bulk and edge states. The corresponding anisotropy Hamiltonian strongly affects the dynamics of the impurity spin at low temperature and voltage and, consequently, changes the results for the edge transport [40].
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