Semiconductors’ sensitivity to electrostatic gating and doping accounts for their widespread use in information communication and new energy technologies. In this Report, I demonstrate quantitatively and with no adjustable parameters that the presence of acceptor dopants explains a variety of hitherto puzzling properties of two-dimensional topological semiconductors at the topological phase transition and in the regime of the quantum spin Hall effect. I exploit the concepts of charge ordering, Coulomb gap, bound magnetic polaron formation, exchange interaction between conducting electrons and holes localized on acceptors, and strong coupling limit of the Kondo effect to explain a short topological protection length, high hole mobilities compared with electron mobilities, and different temperature dependence of the spin Hall resistance in HgTe and (Hg,Mn)Te quantum wells.
Quantized Hall resistance is a hallmark of two-dimensional (2D) topological electronic systems (1). The integer quantum Hall effect’s high-precision quantization is behind a new definition of units (2), whereas other quantum Hall phenomena lead to many far-reaching developments (1). Surprisingly, however, although the quantum spin Hall effect has been known for more than a decade (3–5), experimental resistance magnitudes attain the expected value $h/2e^2$ only in mesoscopic samples, such as micron-size HgTe-based quantum wells (QWs) (6, 7) and sub-100-nm atomically thin 1T’-WTe$_2$ 2D monolayers (8, 9). Moreover, although several theoretical models have been proposed (10), a short experimentally found protection length has usually been assigned (6–9) to unidentified “charge puddles” that trap edge carriers and within which spin-flip, allowing for scattering between helical edges, occurs (11).

I claim here that the challenging properties of quantum spin Hall semiconductors result from the presence of native acceptors in these materials. Accordingly, the starting point for this Report is a quantitative theory of acceptor states in HgTe QWs, which provides positions of acceptor levels with respect to bands and topological edge states as a function of the QW thickness. With this information, I contend that the acceptor density is determined by the gate voltage range in which edge states carry the electric current (5–9, 12, 13). Furthermore, considering charge ordering and Coulomb-gap effects (14), the acceptor scenario explains why at the 2D topological phase transition, the mobility of holes is significantly greater than that of electrons (15, 16), as well as elucidates the origin of high-frequency conductivity (17) and gating hystereses (13). As a next step, I employ a theory of exchange coupling between electrons and acceptor holes (18) to demonstrate that, in topological materials, the interaction between edge electrons with acceptor holes reaches the strong coupling limit of the Kondo effect, where the spin dephasing rate assumes, up to a material-specific logarithmic correction, a universal behavior (19–22). The central result of this Report is that, in this limit, the topological protection length $L_p$ is given by a product of the inverse of one-dimensional (1D) acceptor hole density
in the edge region and the anisotropy of exchange coupling to hole spins. This finding elucidates the magnitude of $L_p$ in HgTe QWs and WTe$_2$ 2D monolayers. Finally, I demonstrate that the formation of acceptor bound magnetic polarons explains a difference in carrier mobilities and the temperature dependence of the edge resistivity of topological HgTe and Hg$_{1-x}$Mn$_x$Te QWs (7).

Native acceptors in compound semiconductors are frequently assigned to metal vacancies giving resulting in double acceptors ($Z = -2$) in II-VI materials, even though the case of ZnTe and CdTe show that residual substitutional impurities, such as Cu ($Z = -1$), are involved (23). To describe acceptor states, a four-band $k \cdot p$ theory developed for acceptors in GaAs and HgTe QWs (24, 25) is extended in this Report to the case, where eight bands are relevant (26), as discussed in detail in supplementary materials (27). Within the axial approximation, the component of the total angular momentum perpendicular the QW plane commutes with the Hamiltonian, meaning that the corresponding integer quantum number $m$ can be used to label acceptor states. For the relevant D$_{2d}$ symmetry and $Z = -1$, the ground-state Kramers doublet corresponds to either $m = 0$ and $m = -1$ or $m = 1$ and $m = -2$. The corresponding binding energies are denoted $E_{1/2}$ or $E_{3/2}$ as the corresponding wave functions are mainly composed of $p_{\pm 1/2}$ and $s_{\pm 1/2}$ or $p_{\pm 3/2}$ Kohn-Luttinger amplitudes, respectively.

Figure 1 depicts energies of relevant QW bands and acceptor ground-state levels for a range of the HgTe QW widths $d_{QW}$ with colors representing a fraction of the $p_{\pm 3/2}$ amplitude in the carrier wave function. Three distinct areas are observed in Fig. 1C: (i) normal band ordering (cation $s$ states above anion $p$ states) at small $d_{QW}$ values; (ii) the range of the topological phase transition centered around the bandgap $E_g = 0$ and $d_c \approx 5.8$ nm; (iii) the topological region $d_w > d_c$, where the band ordering is inverted, resulting in 1D topological gapless edge states (3, 5) to be discussed later. Such a band diagram is generic for this class of 2D topological systems, however the value of $d_c$ depends on strain (set to zero here) and Cd or Mn content in
Figure 1: Band structure and positions of acceptor levels in HgTe QWs of different thicknesses. (A, B) Band energies $E$ vs. wavevector $k$ for unstrained QW thickness of 6 and 8 nm sandwiched between Hg$_{0.3}$Cd$_{0.7}$Te barriers. Red rectangles depict the band region displayed in C. (C) Band edges and acceptor levels (symbols connected by dashed lines vs. QW thickness $d_{QW}$. Except for the orange circles computed for the doubly ionized acceptor ($Z = -2$), other symbols represent the single acceptor ($Z = -1$). The orange symbols ($E_{3/2}$) correspond to acceptors associated with the valence band around $k = 0$; the blue symbols ($E_{1/2}$) with valence band side maxima visible in A and B. Full symbols represent the acceptors residing in the QW center; the open symbols represent acceptors at the distances $d_{QW}/4$, $d_{QW}/2$, and $3d_{QW}/2$ of the QW center. Colors represent the participation of the $p_{\pm 3/2}$ Kohn–Luttinger amplitude in the wave functions.
the barriers and well (15,27).

We note that the binding energies of the doubly ionized acceptors $E^{(2−/−)}$ are irrelevant for the low-energy physics. In contrast, $E^{(−/0)}$ levels, residing near band edges or in the gap, are essential. They originate from either single acceptors ($Z = −1$) or singly ionized double acceptors that, in the mean-field approach, have the same binding energy as single acceptors. As seen in Fig. 1C, in the regions of interest here ($d_{QW} ≈ d_c$ and $d_{QW} > d_c$), the ground state corresponds to the level $E_{1/2}$ associated with the side maximum of the valence band visible in Figs. 1A and 1B. Notably, the acceptor levels form a band, as the hole binding energy depends on the location of the parent acceptor impurity with respect to the QW center, as shown in Fig. 1C.

Within this model, the range of gate voltage corresponding to sweeping over the bandgap $E_g$ at $d_{QW} > d_c$ directly provides the 2D surface density of relevant acceptors $N_s$, with the experimental data implying $N_s ≈ 10^{11}\,\text{cm}^{-2}$ for HgTe QWs (6,16) and $N_s ≈ 10^{13}\,\text{cm}^{-2}$ for WTe$_2$ (8). The value for the acceptor band in HgTe QWs corresponds to the three dimensional (3D) concentration of the order of $N_A = 3 \cdot 10^{16}\,\text{cm}^{-3}$, a typical magnitude for bulk HgTe (28) and Hg$_{1−x}$Mn$_x$Te (29). For such a concentration the holes are localized, as for the evaluated Bohr radius of 5 nm, the Mott critical concentration is $1.4 \cdot 10^{17}\,\text{cm}^{-3}$. Next, I demonstrate that the presence of acceptors explains several hitherto puzzling properties of 2D topological insulators.

One of the rather surprising facts is that low-temperature electron mobility $\mu_e$ in modulation donor-doped HgTe QWs $d_{QW}$ barely reaches $0.4 \cdot 10^6\,\text{cm}^2/\text{Vs}$ (6), whereas $\mu_e$ in bulk HgTe as well as in Hg$_{1−x}$Cd$_x$Te and Hg$_{1−x}$Mn$_x$Te near the 3D topological transition approaches or exceeds $1 \cdot 10^6\,\text{cm}^2/\text{Vs}$ (28–30) with the onset of the Shubnikov de Haas oscillations at 10 mT (29). Even more surprisingly, in the vicinity of the topological phase transition in 2D QWs, the hole mobility $\mu_h$ is larger than $\mu_e$ (15,16), reaching $\mu_h = 0.9 \cdot 10^6\,\text{cm}^2/\text{Vs}$, for which the QHE
Figure 2: **Schematic picture of carrier and acceptor bands at the topological phase transition** ($E_g = 0$). (A) Bulk 3D case with the Fermi energy pinned in the conduction band (c. b.) by acceptors negatively charged below the Fermi level. Coulomb gap at $E_F$ is also shown. (B, C) The same for the 2D case and two positions of the Fermi level. The acceptor band is wide as the binding energy depends on the acceptor location with respect to the QW center.
plateau is resolved in 50 mT in Hg$_{0.976}$Mn$_{0.024}$Te (15), which is relevant for the QHE metrology (16). In addition, the QW hole concentration evaluated from the Hall effect, is significantly smaller than the charge density generated by the gate voltage (15, 16).

Figure 2 elucidates those findings using information obtained from Fig. 1. In the 3D bulk case (Fig. 2A), as previously discussed in detail (14), the acceptor band resides in the conduction band. In addition, due to a small electron mass value, we are on the metallic side of the Anderson–Mott transition so that donors do not bind electrons at any position of the Fermi energy $E_F$. Now, if the donor concentration $N_D \ll N_A$, most of the acceptors are neutral. Furthermore, under these conditions, to reduce the Coulomb energy, only acceptors in close vicinity to donors are ionized. The resulting dipole formation substantially reduces the electron scattering rate. Furthermore, the presence of the Efros–Shklovskii Coulomb gap precludes resonant scattering. By fine hydrostatic pressure tuning of the band structure toward the 3D topological transition at $E = 0$, $\mu_e = 20 \cdot 10^6$ cm$^2$/Vs was registered in Hg$_{0.94}$Mn$_{0.06}$Te at 2 K (29).

The situation is entirely different at the topological phase transition in the 2D case. As shown in Fig. 2B, for the Fermi level in the conduction band, obtained through modulation donor doping, all acceptors are ionized, explaining the low electron mobility. In contrast, in the hole transport regime (Fig. 2C), achieved by gating-induced discharging of acceptors, the aforementioned charge ordering occurs, which along with the small effective mass of holes in the Dirac cone and the formation of the Coulomb gap $E_C$, results in high hole mobilities at $k_B T < E_C \approx 0.3$ meV (27). Higher carrier mobility in Mn-containing samples (15, 29) compared to the HgTe case may not be accidental: $E_C$ is enlarged by the acceptor bound magnetic polaron (BMP) energy $E_p$, where for $x_{Mn} = 0.02$, $E_p > 0.3$ meV at $T < 2$ K (27). The Coulomb gap model explains also a large thermal stability of the QSHE in WTe$_2$ (9, 27).

Having elucidated the role of acceptors in the region of the topological phase transition we focus on the region $d_{QW} > d_c$ (Fig. 2C). Here, the Coulomb gap diminishes d. c. hoping conduc-
tivity. However, since there is no Coulomb gap for electron–hole excitations, the presence of the acceptor band explains the origin of puzzling gap states detected by high-frequency conductivity (17). Moreover, under these conditions, one can anticipate the appearance of the exchange interaction $\mathcal{H}_{eh}$ between spins of electrons in the topological edge states, $s$, and acceptor holes, $J$.

To reveal the striking consequences of this suggestion, I recall that a long-range component of this coupling originates from the virtual radiative recombination of electron–hole pairs, for which the exchange energy $\mathcal{J}_{eh} \propto 1/E_{eh}^2$, where $E_{eh}$ represents the electron–hole energy distance. According to the theory (18, 27), which is quantitatively verified for the interaction between band edge electrons and holes on Mn acceptors in GaAs (32), $\mathcal{H}_{eh} = -\mathcal{J}_{eh} s \cdot J$, where $J = 3/2$ and $\mathcal{J}_{eh} = -0.23$ eV (18). When $E_{eh} = 1.4$ eV in GaAs:Mn, the lower bound of $E_{eh}$ is as small as $E_C \approx 0.3$ meV for the topological edge electrons and acceptor holes. Hence, the antiferromagnetic $\mathcal{J}_{eh}$ is the largest relevant energy, and despite a small DOS magnitude at $E_F$ in semiconductors, drives the system to a strong coupling limit of the Kondo effect, specified in QWs by a wide distribution of Kondo temperatures $T_K$. Importantly, for the parameter values expected for HgTe QWs, i.e., the Fermi velocity $v_F = 4 \cdot 10^5$ m/s, the penetration length of the edge electron wave function into the QW, $b = 7$ nm, and $N_s = 10^{11}$ cm$^{-2}$, the number of edge electrons per unit length for $E_F$ in the gap center $N_e = E_g/2\pi \hbar v_F = 12/\mu$m is greater than the number of acceptor holes in the edge region, $N_h = N_s b/2 = 4 \mu$m. This would also be the case of the double acceptors for which, if the Hund’s rule is obeyed, $N_h = N_s b/2$, independently of $E_F$. Thus, we can quantitatively verify numerous theoretical studies on the Kondo effect in QSHE materials, developed originally for systems doped with magnetic ions (19–21).

More specifically (27), since the edge states break the axial symmetry,

$$\mathcal{H}_{eh} = -\mathcal{J}_x s_x j_x - \mathcal{J}_y s_y j_y - \mathcal{J}_z s_z j_z,$$

(1)
Figure 3: **Destructive role of charge dopants in the quantum spin Hall effect.** If axial symmetry is maintain ($J_x = J_y$) only spin-flop ($\uparrow\downarrow \leftrightarrow \downarrow\uparrow$) transitions occur (case 1 in the figure), so that edge current is conserved in the spin–momentum locking situation. However, if $J_x \neq J_y$, $\uparrow\uparrow \leftrightarrow \downarrow\downarrow$ spin nonconserving transitions are also allowed (case 2), leading to net backscattering after a chain of spin-dependent interactions of electrons with an acceptor.
where \( j = 1/2 \) for a singly occupied acceptor and the relevant ground state \( E_{1/2} \). For helical states with spin–momentum locking, exchange anisotropy ensures the leak of electron spin momentum to crystal orbital momentum in a chain of scattering events, resulting in net carrier backscattering \((20, 21, 27)\), as sketched in Fig. 3 \((20, 21, 27)\). The resulting backscattering rate, compared to the conventional spin dephasing rate \( \gamma_m \), is reduced by a factor \( r = \frac{2(J_x - J_y)}{(J_x + J_y)^2} \) \((20, 21, 27)\).

In terms of the edge electron dwell time \( L_x/v_F \) and \( r\gamma_m \), the topological protection length \( L_p = v_F/r\gamma_m \). Making use of the \( \gamma_m \) form determined by the Wilson’s numerical renormalization group approach in the Kondo regime \((22)\), we obtain the main finding of this Report,

\[
L_p = 1.0/[N_h r F(T/T_K)],
\]

where \( F(x) = 1 \) at \( x = 1 \), it decays to zero at \( x \to 0 \) and slowly decreases with \( x \) for \( x > 1 \) (for \( x = 0.2 \) and 10, \( F(x) = 0.5 \) and 0.6, respectively) \((22)\). For parameters typical to topological HgTe QWs, i.e., \( d_{QW} = 8 \text{ nm} = 0.05 \text{ nm}^{-1} \), \( b = 7 \text{ nm} \), the effective in-plane Bohr radius \( a^* = 5 \text{ nm} \), and the acceptor distance to the edge \( y_d = 7 \text{ nm} \), we obtain \( r = 2 \cdot 10^{-2} \) \((27)\). Thus, for \( N_h = 4/\mu \text{m} \), Eq. 2 implies \( L_p = 13 \mu \text{m} \) at \( T = T_K \), the magnitude falling within the range of the observed values \((13)\). This is also the case of WTe\(_2\) in which \( N_s = 10^{13} \text{ cm}^{-2} \) and \( b = 2 \text{ nm} \) \((8, 31)\), so that \( N_h = 10^2 \mu \text{m} \), resulting in \( L_p = 0.5 \mu \text{m} \) following the experimental data \((8, 9)\).

An unexpected appearance of quantized resistance below 0.3 K in a Hg\(_{0.988}\)Mn\(_{0.012}\)Te QW \((7)\) can be elucidated using the acceptor model by spin splitting \( \Delta \) of hole states originating from the BMP effect, as for \( x = 0.012 \), \( \Delta > k_B T \) at \( T < 5 \text{ K} \) \((27)\). Interestingly, the existing theories on the disappearance of the Kondo effect in a magnetic field assume the same \( \Delta \) for the impurity and band states \((33)\), which is not the case in the presence of BMPs.

Furthermore, a small number of holes and acceptors involved leads to reproducible resis-
tance fluctuations (5, 7–9). At the same time, filamentary charging and discharging of barrier acceptors under a strong gate electric field may account for hystereses and irreversibilities in low-temperature transport properties when cycling the gate voltage (7, 13).

In summary, the proposed acceptor impurity band model can elucidate the critical properties of QSHE materials. In this Report, the model’s quantitative predictions have been compared to experimental data on HgTe and Hg$_{1-x}$Mn$_x$Te QWs as well as on 1T’-WTe$_2$ 2D monolayers, however, it would be interesting to verify the model in the case of other QSHE candidate materials, such as α-Sn and Bi films, other 2D monolayers, and Heusler compounds with an inverted band structure. More generally, while electrostatic gating is widely used to reveal the unique properties of quantum materials, the results presented here demonstrate that charge dopants play an important and unanticipated role in the physics and applications of topological semiconductors.
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Supplementary materials

Materials and Methods

Figs. S1 - S3

References (34 - 50)

S1 Quantum well band states

A starting point of our theory is the eight-band Kohn–Luttinger Hamiltonian with boundary conditions previously used in obtaining the subband structure in HgTe QWs (26) and the four–band model developed for determining, in the axial approximation, acceptor levels in GaAs QWs (24). Within that approximation, discussed in Sec. S2, and in the absence of the impurity potential, the eight relevant electron wave functions $\psi_j$ can be taken in the form,

$$\psi_j(\rho, \varphi, z) = f_j(\rho, \varphi) h_j(z) u_j,$$  \(S1\)

where $\rho$, $\varphi$, and $z$ denote the electron position in the cylindrical coordinates with $z$ along the growth direction; $u_j$ is the set of the Kohn–Luttinger amplitudes: $s_{1/2,1/2}$, $s_{1/2,-1/2}$, $p_{3/2,3/2}$, $p_{3/2,1/2}$, $p_{3/2,-1/2}$, $p_{3/2,-3/2}$, $p_{1/2,1/2}$, and $p_{1/2,-1/2}$, whereas the envelope functions $f_j(\rho, \varphi)$ and $h_j(z)$ are given by,

$$f_j(\rho, \varphi) = N_o i^{\lfloor m_j \rfloor} \exp(i m_j \varphi) J_{\lfloor m_j \rfloor}(k\rho),$$  \(S2\)

where $N_o$ is a normalization factor, $m_j = m$ for $j = 1, 4,$ and $7$; $m_j = m + 1$ for $j = 2, 5,$ and $8$; $m_j = m - 1$ for $j = 3$, and $m_j = m + 2$ for $j = 6$; $m$ is the integer orbital quantum number; $J_{\lfloor m_j \rfloor}(k\rho)$ is the Bessel function; $k$ is a module of the in-plane wavevector, and

$$h_j(z) = (1/L_z)^{1/2} \sum_{n=-n_{\text{max}}}^{n_{\text{max}}} c_n^{(j)} \exp(2\pi in z/L_z),$$  \(S3\)
where $L_z$ is the total width of the structure, including the two \text{Cd}_{0.7}\text{Hg}_{0.3}\text{Te}$ barriers and HgTe QW, assumed here as $L_z = 60\, \text{nm} + d_{\text{QW}}$; the expansion coefficients $c_n^{(j)}$ are to be determined by a diagonalization procedure; $n_{\text{max}} = 25$ ensures an appropriate numerical convergence, as discussed in Sec. S4.

We adopt the identical values of $k \cdot p$ parameters, as in Ref. (26), except for the Luttinger $\kappa$ that we assume to be the same in the barriers and QW. In this way, no Rashba-like splitting occurs in symmetric QWs. Computations have been performed assuming the absence of strain. Its role is discussed in Sec. S3.

\section*{S2 Axial approximation}

Figure S1 shows subband dispersions $E(k)$ computed without and with the axial approximation of a HgTe QW. As the energy differences between $k_\parallel \langle 10 \rangle$ and $k_\parallel \langle 11 \rangle$ near valence band top are significantly smaller than the acceptor binding energies in Fig. 1, the axial approximation holds.

\section*{S3 Strain effects}

We use a conventional sign definition of biaxial epitaxial strain (34–36), i.e., a positive value of $\epsilon_{xx} = \epsilon_{yy}$ corresponds to QW under the tensile strain. In particular, in the case of HgTe QW, $\epsilon_{xx} = 0.31\%$ corresponds to strain for a CdTe substrate, whereas a Cd$_{1-x}$Zn$_x$Te substrate generates a compressive strain (37), $\epsilon_{xx} < 0$. The evolution of the QW band structure with biaxial strain is shown in Fig. S2 for HgTe QW of the thickness $d_{\text{QW}} = 6\, \text{nm}$ and $\epsilon_{xx} = 0.31\%, 0$, and $-0.31\%$. The strain shifts the QW thickness corresponding to the topological phase transition ($E_g = 0$), but the overall band picture remains intact, in agreement with previous conclusions (26, 37).
Figure S1: Verification of axial approximation. Subband dispersions for a HgTe QW of the thickness $d_{QW} = 6$ nm computed for $k \parallel \langle 11 \rangle$ (dotted lines), $k \parallel \langle 11 \rangle$ (dashed line) and within the axial approximation (solid line).
Figure S2: Effects of biaxial strain on band dispersion in HgTe QW. (A) $\epsilon_{xx} = 0.31\%$ (CdTe substrate); (B) $\epsilon_{xx} = 0$; (C) $\epsilon_{xx} = -0.31\%$. Colors describe the participation of the $p_{3/2, \pm 3/2}$ Kohn-Luttinger amplitude in the electronic wave function; HgTe QW thickness $d_{QW} = 6$ nm.
To determine energies of levels brought about by charge dopants, we supplement the Hamiltonian by the Coulomb potential,

\[ V(r) = -Z e^2 / 4\pi\varepsilon_0 \varepsilon_r, \]  

(S4)

and by the potential of image charges in the barriers (24), for which the dielectric constant is 

\[ \varepsilon_b = (1 - x_b)\varepsilon + x_b\varepsilon_e, \]

where in our case \( \varepsilon = 19.5, \varepsilon_e = 10.5, \) and \( x_b = 0.7. \) We neglect central cell corrections and the image charge in the gate metal, which is typically more than 100 nm apart.

Furthermore, we replace the Bessel function \( J_{|m_j|}(k\rho) \) in Eq. S2 by

\[ J_{|m_j|}(k\rho) \rightarrow \rho^{|m_j|} \sum_{l=1}^{l_{\text{max}}} d_l^{(j)} \exp(-\rho/a_l), \]  

(S5)

where the coefficients \( d_l^{(j)} \) are to be determined by the diagonalization procedure for given values of \( a_l. \) We take \( a_l \) as a geometrical series with a common ratio of \( r = 1.5 \) and, for a typical number of exponential functions \( l_{\text{max}} = 15, \) the starting value of \( a_1 = 0.5 \) nm. Since, the exponential functions with real exponents are not orthogonal, a generalized eigenvalue solver has been employed to obtain electronic energies. At the same time, the participation number serves to evaluate an effective in-plane localization radius \( a^*. \)

The presence of the impurity potential breaks the degeneracy of the states with respect to the quantum number \( m. \) However, due to time-reversal symmetry, the impurity levels remain at least doubly degenerate. The use of exponential functions (Eq. S6) is suitable for determining the localized levels but not for oscillating extended states. Accordingly, the values of band energies do not converge with increasing \( l_{\text{max}}. \)

In our case, identifying acceptor levels that overlap with the continuum of band states appears difficult (38, 39). Figure S3 depicts level energies \( i \) determined for \( m = 1 \) in a HgTe
Figure S3: Example of the identification of acceptor levels $E_{3/2}$ ($m = 1$) degenerate with the QW band states. (A) Energy levels $E$ as a function of the center charge $Z$. (B) $E$ as a function of the number of exponential functions $l_{\text{max}}$ in Eq. S6 and for $n_{\text{max}} = 25$ (Eq. S3). (C) $E$ as a function of the distance of acceptor to QW center $z_0$ for $l_{\text{max}} = 15$ and $n_{\text{max}} = 50$. Color scale depicts the magnitude of an effective in-plane Bohr radius $a^*$ in the logarithmic scale. Red solid lines show the ground state $E_{3/2}$ acceptor level; dotted lines represent examples of acceptor excited states. HgTe QW thickness $d_{\text{QW}} = 6$ nm; no strain.
QW with \( d_{\text{QW}} = 6 \text{ nm} \). As shown, the magnitude of \( a^* \), and the evolution of the level energies with \( Z \) (Fig. 3A), \( l_{\text{max}} \) (Fig. 3B), and with the acceptor location of the QW center (Fig. 3C) unambiguously tell the band and resonant impurity states.

**S5 Coulomb gap**

The Efros-Shklovskii Coulomb gap \((40)\) of the width \( E_C \) reaching 10 meV was observed in a single-layer of 1T'-WTe\(_2\) with different coverage of surface by potassium \((41)\). Furthermore, numerical simulations revealed the presence of the Coulomb gap for resonant donor states in HgSe:Fe \((14)\).

In terms of 2D DOS of the acceptor band taken as \( \nu_2 = N_s/E_b \), where \( E_b \) is the acceptor bandwidth \((40)\),

\[
E_C = 2\nu_2 e^4/(4\pi\epsilon_0\epsilon)^2. \tag{S6}
\]

For HgTe QW, where \( N_s = 10^{11} \text{ cm}^{-2} \); \( E_b = 30 \text{ meV} \), and the QW dielectric constant \( \epsilon = 19.5 \), the magnitude of \( E_C = 0.34 \text{ meV} \). This value sets the temperature scale above which the hole mobility \( \mu_h \) decreases and conductance quantization deteriorates. Thus, the Coulomb gap model explains the stability of the QSHE up to 100 K in WTe\(_2\) monolayers \((9)\), where – as mentioned above – \( E_C \) attains 10 meV \((41)\).

**S6 Magnetic polaron gap and zero-field spin-splitting**

We consider isoelectronic magnetic impurities, such as Mn in II-VI compounds, in the paramagnetic phase. The presence of \( sp-d \) exchange interactions affect charge dopants even in the absence of macroscopic magnetization by the bound magnetic polaron (BMP) effect. Optical studies provided the evidence for the presence of the acceptor BMP in Hg\(_{1-x}\)Mn\(_x\)Te \((42,43)\). A contribution of the BMP to thermally activated band conductivity \((44)\) and to the Coulomb gap
in the hoping region (45) was found in Cd$_{1-x}$Mn$_x$Te.

According to the analytical solution of the central spin problem, the polaron energy $\epsilon_p$ determines BMP energetics and thermodynamics in the absence of an external magnetic field (46),

$$\epsilon_p(T) = \mathcal{J}_{sp-d}^2 \chi_{Mn}(T)/[32(g_{Mn}\mu_B N_0)^2\pi a_B^3],$$  \hspace{1cm} (S7)

where the magnitude of the exchange energy $\mathcal{J}_{sp-d}$ is given here by the values of the $s-d$ and $p-d$ exchange integrals [$N_0\alpha = 0.3\text{ eV}$ and $N_0\beta = -0.7\text{ eV}$ for Hg$_{1-x}$Mn$_x$, respectively (47)], contributing proportionally to the corresponding orbital content of the acceptor wave function; $\chi_{Mn}(T)$ is the Mn susceptibility in the absence of acceptors; $g_{Mn} = 2.0$; the cation concentration $N_0 = 1.49 \cdot 10^{22}\text{ cm}^{-3}$, and $a_B$ is the acceptor localization radius determined from the participation number. In the case of the doubly occupied acceptor with $J = 1$, $\epsilon_p(T)$ would be four times greater.

We identify the polaron gap between occupied and non-occupied acceptor centers, $E_p$, as the twice Fermi energy shift associated with the polaronic effect. For the doubly degenerate acceptor state $E_p$ assumes the form (44),

$$E_p = \epsilon_p + 2k_B T \ln(1 + \epsilon_p/k_B T).$$  \hspace{1cm} (S8)

For the $E_{3/2}$ state, $\mathcal{J}_{sp-d} = -0.7\text{ eV}$ implying $E_p = 2.6\text{ meV}$ at $T = 2\text{ K}$, $x = 0.02$, and $a_B = 4\text{ nm}$. Similarly, for the more relevant $E_{1/2}$ case, $\mathcal{J}_{sp-d} = -0.2\text{ eV}$, for which $E_p = 0.35\text{ meV}$. For the $x$ value in question there are about 500 Mn ions within the volume visited by the acceptor hole. We conclude that the formation of BMPs in Hg$_{1-x}$Mn$_x$ may substantially enhance the magnitude of the gap at the Fermi level in the acceptor band compared to the case of HgTe.

In the case of the Kondo effect we are interested in the magnitude of acceptor hole spin-splitting. Depending on temperature, the most probable magnitude of zero-field splitting $\bar{\Delta}$ is
given by (46),

\[ \bar{\Delta} = 2\epsilon_p(T) + 4k_B T \text{ for } \epsilon_p(T) \gg k_B T; \quad (S9) \]

\[ \bar{\Delta} = 2[2\epsilon_p(T)k_B T]^{1/2} + 8^{1/2}\epsilon_p(T) \text{ for } \epsilon_p(T) \ll k_B T. \quad (S10) \]

For the parameters quoted above we obtain \( \bar{\Delta} = 5 \text{ meV} \) and 0.9 meV for the \( E_{3/2} \) and \( E_{1/2} \) level, respectively. In the particular case of the sample with \( x = 0.012 \) studied in Ref. (7) and for the level \( E_{1/2} \), \( \bar{\Delta} = k_B T \) at \( T = 5 \text{ K} \). It is clear that the presence of BMPs may have a significant influence on the Kondo effect at low temperatures.

**S7 Evaluation of the electron-hole spin exchange**

We are interested in determining the degree \( r \) of axial symmetry breaking by the QW edge for the exchange interaction between topological edge electrons and acceptor holes in HgTe QWs. Our starting point is the Bir–Pikus theory developed for excitons (34), and later extended to the case of exchange coupling between band electrons and acceptor holes in bulk semiconductors (18). Since the QW and edge states break the rotational symmetry \( \mathcal{H}_{eh} \) can assume, in the presence of spin-orbit coupling, a general non-scalar form, \( \mathcal{H}_{eh} = -\sum_{\alpha,\beta}s_\alpha j_{\alpha\beta} \) that allows for the pseudo-dipole and Dzyaloshinskii-Moriya terms.

We consider the long-range contribution that scales to the strong coupling limit and use the identity separating the interaction into the monopole and dipole contribution,

\[ \frac{\partial^2}{\partial r_{1,\alpha} \partial r_{2,\beta}} \frac{1}{r_{12}} = -\frac{4\pi}{3} \delta_{\alpha,\beta} \delta(r_{12}) - \frac{r_{12}^2 \delta_{\alpha,\beta} - 3r_{12,\alpha} r_{12,\beta}}{r_{12}^5}, \quad (S11) \]

where \( r_{12} = r_1 - r_2 \) and \( \alpha, \beta = x, y, z \).

Since the acceptor ground-state in the topological regime composes in 85% of \( p_{3/2, \pm 1/2} \) for \( m = 0 \) and \( m = -1 \), respectively, we neglect other contributions to the hole wave function.
Under these assumptions, we obtain \( H_{eh} = - \sum_\alpha \mathcal{J}_\alpha s_\alpha j_\alpha \), where

\[
\mathcal{J}_{x,y} = A \left( \frac{16\pi}{9} I_{11c} + \frac{4}{3} I_{12cp} \pm I_{12acp} \right); \quad \mathcal{J}_z = A \left( \frac{8\pi}{9} I_{11} + \frac{5}{3} I_{12cm} \right). 
\]

Here

\[
A = -|e_s|^2 |h_{12}|^2 \frac{e^2}{4\pi\epsilon_0 \epsilon} \frac{P^2}{E_{eh}^2},
\]

where \(|e_s|^2\) and \(|h_{12}|^2\) denote a fractional contribution of the \( s_{1/2,1/2} \) and \( p_{3/2,1/2} \) Kohn–Luttinger amplitudes to the edge electron and QW hole wave function, respectively; \( P \) is Kane’s \( s-p \) momentum matrix element; \( I_s \) represent matrix elements over the monopole and dipole contributions, involving electron \( F_e(r) \) and hole \( F_h(r) \) envelope functions, assumed – for the states in question – in the form, \( F_e(r) = \exp(ikx) f_e(r) / \sqrt{L_x} \), where \( L_x \) is the edge channel length and

\[
f_e(r) = \exp(-y/b) \Theta(y) \cos(\pi z / d_{QW}) \Theta(d_{QW}/2 - |z|)/(b/2)^{1/2}; \\
F_h(r) = \exp(-[x^2 + (y - y_0)^2]^{1/2} / a^*) \Theta(y) \cos(\pi z / d_{QW}) \Theta(d_{QW}/2 - |z|) / N_o.
\]

Here \( b \) describes the penetration length of edge electrons into the QW; \( \Theta(x) \) is the Heaviside step function, \( y_0 \) is the distance of the parent acceptor to the edge located at \( y = 0 \), and \( N_o \) is a normalization factor.

It is convenient to introduce a general integral \( I \) and integrand functions \( g(r_1, r_2) \) that are different for particular matrix elements \( I_s \),

\[
I = \int dr_1 dr_2 g(r_1, r_2) f_e(r_1) F_h(r_1) f_e(r_2) F_h(r_2),
\]

where for \( I_{11}, I_{11c}, I_{12cp(m)}, \) and \( I_{12acp} \), \( g(r_1, r_2) = \delta(r_{12}); \cos[k(x_1 + x_2)] \delta(r_{12}); \cos[k(x_1 \pm x_2)] (r_{12}^2 - 3z_{12}^2)/r_{12}^5; \cos[k(x_1 + x_2)] (x_{12}^2 - y_{12}^2)/r_{12}^5 \), respectively.
Results of Refs. (20,21) lead to the reduction factor \( r = \left[2(\mathcal{J}_x - \mathcal{J}_y)/(\mathcal{J}_x + \mathcal{J}_y)\right]^2 \) for \( r \ll 1 \).

The magnitude of \( r = 2 \cdot 10^{-2} \) quoted in the main text has been evaluated for \( b = 7 \) nm (48–50), \( d_{QW} = 8 \) nm, \( k = 0.05 \) nm\(^{-1}\), \( a^* = 5 \) nm, \( b = 7 \) nm, and \( y_0 = 7 \) nm.
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