Tunable quantum spin Hall effect in double quantum wells

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The field of topological insulators (TIs) is rapidly growing. Concerning possible applications, the search for materials with an easily controllable TI phase is a key issue. The quantum spin Hall effect, characterized by a single pair of helical edge modes protected by time-reversal symmetry, has been demonstrated in HgTe-based quantum wells (QWs) with an inverted bandgap. We analyze the topological properties of a generically coupled HgTe-based double QW (DQW) and show how in such a system a TI phase can be driven by an inter-layer bias voltage, even when the individual layers are non-inverted. We argue, that this system allows for similar (layer-)pseudospin based physics as in bilayer graphene but with the crucial absence of a valley degeneracy.

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Since the understanding of the topological nature of the quantum Hall effect1,2,3,4,5 topological phases have become one of the most active research fields in condensed matter physics. More recently, a new topological phase preserving time-reversal symmetry (TRS), the quantum spin Hall (QSH) phase, has been discovered. The QSH phase has been theoretically predicted5 and experimentally realized in 2D HgTe/CdTe QWs.6 The crucial ingredient of this narrow gap semiconductor material is strong spin-orbit coupling, which determines the inverted band structure of HgTe. The experimentally accessible parameter tuning the band structure from normal (CdTe-like) to inverted is the thickness of the HgTe QW. One year later, 3D TIs supporting chiral fermions as surface states have been proposed and observed7–12. These two phenomena are examples of the general concept of a TI which is a TRS preserving system with a bulk insulating gap which features topologically protected edge states due to the Atiyah-Singer index theorem which is in this context referred to as the bulk boundary correspondence. TI phases are characterized by a $\mathbb{Z}_2$ topological invariant.3,13

In this work, we extend the Bernevig-Hughes-Zhang (BHZ) model1 to account for a double QW (DQW) of HgTe (see Fig. 1). We analyze how the topological features of the DQW depend on a generic coupling Hamiltonian effectively connecting the two wells and on the applied voltage $V$ between them. In particular, we show that a QSH phase can be driven by $V$ also when the two QWs are individually trivial. We also derive a reduced 2-band model that well captures the topological features of the system. We give analytical expressions of the effective parameters that map the reduced model to the BHZ-model of a single HgTe QW [in Eq. (10)] as a function of the tunneling matrix elements and voltage $V$. We show that a non-trivial $\mathbb{Z}_2$ topological invariant is accompanied with the appearance of a single pair of helical edge states for which we calculate the energy dispersion and spinors. In Fig. 2(a) we show the phase diagram of the model as a function of tunneling amplitude and applied voltage.

![FIG. 1: (Color online) (a) Schematic representation of the HgTe/CdTe DQW made by a front and back well with a finite overlap of their individual envelope functions $\chi_f(z)$ and $\chi_b(z)$ as shown in (b). (c) Process of band inversion in a DQW caused by a potential bias.](image)

I. DOUBLE QUANTUM WELL MODEL

The system under investigation consists of a DQW of HgTe as shown in Fig. 1, which can be thought of as a 2D TI bilayer. The system is contacted to gates that control the potential bias $V$ between the front (f) and back (b) QWs. The spectrum of a single HgTe-based QW near the $\Gamma$-point is effectively described by the BHZ model:

$${H}_0 = \begin{pmatrix} h(\vec{k}) & 0 \\ 0 & h^*(\vec{-k}) \end{pmatrix}$$

$$h(\vec{k}) = \vec{\alpha} \cdot \vec{\sigma}$$

$$\vec{\alpha} = (C - D\vec{k}^2, Ak_x, -Ak_y, M - B\vec{k}^2),$$

where $\vec{k}$ is the wavevector in the plane of the QW, $C$ is the confinement energy, $D$ is the gap parameter, $A$ and $B$ are the spin-orbit coupling parameters, and $M$ is the mass of the hole. The Hamiltonian $H_0$ is in the mass basis, and $h(\vec{k})$ is the Dirac Hamiltonian in the presence of the applied electric field $\vec{E}$.

The bulk sector of the Hamiltonian is diagonalized by the momentum $\vec{k}$, while the edge sector is described by the pseudospinors $\psi_f(z) = \chi_f(z) + \chi_b(z)$ and $\psi_b(z) = \chi_f(z) - \chi_b(z)$, where $\chi_f(z)$ and $\chi_b(z)$ are the envelope functions of the frontier and backwell, respectively. The Hamiltonian in the presence of the applied voltage $V$ is given by:

$${H} = {H}_0 + \frac{eV}{\hbar} \vec{A}(z) \cdot \vec{\sigma}$$

where $\vec{A}(z)$ is the electric field, which is a function of the position $z$. The electric field $\vec{A}(z)$ is given by:

$$\vec{A}(z) = \begin{pmatrix} 0 \\ 0 \\ -U(z) \end{pmatrix}$$

where $U(z)$ is the applied voltage.

The edge sector of the Hamiltonian is diagonalized by the momentum $\vec{k}$ and the pseudospin $\vec{\sigma}$, which leads to the following dispersion relations:

$$E_{\vec{k}} = \pm \sqrt{h^2(\vec{k}) + \frac{e^2}{\hbar^2} U(z)^2}$$

where $E_{\vec{k}}$ is the energy of the edge state.

The edge states are protected by TRS and have a chirality which is determined by the direction of the applied voltage. The chirality is given by:

$$\chi = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The chirality is a function of the momentum $\vec{k}$ and the pseudospin $\vec{\sigma}$.

In the presence of the applied voltage $V$, the edge states are split into two sets, one with positive chirality and the other with negative chirality. The positive chirality states are shifted to lower energy, while the negative chirality states are shifted to higher energy.

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where \( \hat{\sigma} \) are the Pauli matrices\(^{14}\) associated with the band-pseudospin degree of freedom (band \( E_1 \) or \( H_1 \)). \( H_0 \) is represented in the basis \( \{ |E_1\rangle, |H_1\rangle, |E_1\rangle, |H_1\rangle \} \), where the \( E_1 \) states \( (J_z = \pm 1/2) \) are a mixing of the s-like \( \Gamma_6 \) band with the \( \Gamma_8 \) light-hole band, while \( H_1 \) \( (J_z = \pm 3/2) \) is basically the \( \Gamma_8 \) heavy-hole band\(^{15}\). In the following we will use the parameter values \( A = 375 \) meV nm, \( B = -1.120 \) eV nm\(^2\) and \( D = -730 \) meV nm\(^2\), estimated by a comparison with the \( 8 \times 8 \) Kane Hamiltonian\(^{16}\), and assume \( C = 0 \) without loss of generality. The Dirac rest mass \( M \) depends on the QW thickness and \( M < 0 \) corresponds to the inverted (QSH) regime whereas \( M > 0 \) corresponds to the normal regime. In first approximation, \( H_0 \) is block diagonal in the Kramer’s partner or spin degree of freedom\(^{18}\) (with \( \vec{\sigma} \) the vector of Pauli matrices). Because we consider only systems with TRS, we restrict ourselves to the block \( h(\vec{k}) \), from which the results can be extended to the other one by applying the time reversal operator \( \hat{T} = i\vec{\sigma} \vec{k} \).

The Hamiltonian \( h(\vec{k}) \) in Eq. (1) describes the in-plane electronic motion inside a QW layer. Along the confinement direction of the QW \( (Z) \), electrons are described by the envelope function \( \chi_0(z) \) (integrated out in the BHZ model). When the two QWs of a DQW are sufficiently separated, an electron will be localized either on the f or on the b layer, with envelope function \( \chi_0^f(z) \) and \( \chi_0^b(z) \), resp. When the two layers are placed close to each other, \( \chi_0^f(z) \) and \( \chi_0^b(z) \) acquire a finite overlap, accounted for by a tunneling Hamiltonian \( H_T \). This description should take into account that \( \chi_0(z) \) is a spinor with components on the \( E_1 \) and \( H_1 \) bands. To first order in \( k \), the tunneling Hamiltonian has the form

\[
H_T = \frac{\mathcal{R} (\hat{\Delta}) \cdot \hat{\sigma}}{2} P_x - \frac{\mathcal{I} (\hat{\Delta}) \cdot \hat{\sigma}}{2} P_y \tag{2}
\]

where \( P_i \) are Pauli matrices associated with the layer projection \( \{ \text{layer pseudospin (LPS) } \vec{P} \} \). \( H_T \) generates bonding/antibonding states with energy splitting \( \Delta_{E1} = \Delta_0 + \Delta_z \) \( (\Delta_{H1} = \Delta_0 - \Delta_z) \) of the \( E1 \) \( (H1) \) band. The lowest order off-diagonal term is \( \alpha k_x \), due to the axial symmetry and the \( J_z \) character of \( E1 \) and \( H1 \) bands\(^{15}\). In the Appendix A, we present a realistic estimate of HgTe DQW tunneling parameters.

The DQW Hamiltonian for a single Kramer’s block is therefore

\[
H = \hat{d} \cdot \hat{\sigma} P_0 + \frac{\mathcal{R} (\hat{\Delta}) \cdot \hat{\sigma}}{2} P_x - \frac{\mathcal{I} (\hat{\Delta}) \cdot \hat{\sigma}}{2} P_y + \frac{1}{2} (\delta \hat{d} \cdot \hat{\sigma}) P_z, \tag{3}
\]

where \( \delta \hat{d} \) is due to the possible variation of the parameters of \( h(k) \) between the f and the b layer. In particular, we consider \( \delta \hat{d} = (V, 0, 0, 0) \), with \( V \) the interlayer bias.

**II. BAND STRUCTURE AND TOPOLOGY**

The topological properties of a fully gapped 2D TRS preserving system are described by the \( \bm{Z}_2 \)-invariant \( \nu \). When the model Hamiltonian is block diagonal with respect to the Kramer partner spin \( \vec{s} \), the system can be thought of, from a topological point of view, as two copies of an anomalous quantum Hall effect, related by time reversal\(^{15}\). Each of the blocks is topologically characterized by its first Chern number \( C_1 \) and \( C_1 \) resp., which we call the Kramers Chern numbers (KCNs). TRS immediately implies that the two KCNs obey a zero sum rule\(^{16}\), meaning \( C_1 = -C_1 \). The \( \bm{Z}_2 \) invariant is then given by\(^{15}\)

\[
\nu = \frac{C_1 - C_1}{2} (\text{mod } 2) = C_1 (\text{mod } 2), \tag{4}
\]

with the KCN defined as

\[
C = \frac{i}{2 \pi} \int_{\mathbb{T}^2} \mathcal{F}, \tag{5}
\]

and where the Berry curvature is given by

\[
\mathcal{F}(k) = \sum_{\alpha \text{ occ}} (d(u_{\alpha}^k)) \wedge (d(u_{\alpha}^k)), \tag{6}
\]

where \( \wedge \) stands for the exterior product. The sum is over the occupied bands and \( |u_{\alpha}^k\rangle \) are Bloch states of the Kramers block Hamiltonian. In order to make the Chern number well defined in local models, like Eq. (3) a lattice regularization has to be included to compactify the \( k \)-space. In our case, since the curvature decays rapidly away from the \( \Gamma \)-point, the integral in Eq. (5) over the \( k \)-space \( \mathbb{R}^2 \) converges stably towards the KCN of the lattice regularized model.

Let us first analyze the bulk dispersion curves described by Eq. (3) to get an intuition for possible local topological phase transitions\(^{20}\) at the \( \Gamma \)-point, induced by band crossings. For \( k = 0 \) we obtain the four eigenenergies

\[
E_{\pm}(0) = \eta M \pm \frac{1}{2} \sqrt{\left(\Delta_0 + \eta \Delta_z\right)^2 + V^2}, \tag{7}
\]

with \( \eta = \pm 1 \). Due to the interlayer tunneling, the \( E1 \) bands (centered at \( E = M \)) suffer an energy splitting, at the \( \Gamma \)-point, of \( \sqrt{\Delta_{E1}^2 + V^2} \), while for the \( H1 \) bands (centered at \( E = -M \)) the splitting is \( \sqrt{\Delta_{H1}^2 + V^2} \). We define a local energy gap (LEG) at \( k = 0 \) as

\[
E_g(0) = 2M \text{sgn}(M) \left( \sqrt{\Delta_{E1}^2 + V^2} + \sqrt{\Delta_{H1}^2 + V^2} \right). \tag{8}
\]

When the LEG changes sign an inversion of bands with \( E1 \) and \( H1 \) character occurs at the \( \Gamma \)-point, accompanied by a possible topological phase transition. For a fixed set of parameters, the condition \( E_g(0) = 0 \) defines (if existent) the critical value of the bias \( V_c \) driving the phase
Interestingly, for time-reversal protected helical modes. An example of the DQW is topologically non-trivial and allows for a pair of small $|\alpha|$ calculated the KCN invariant with Eq. 4, as shown in Fig. 2, where we numerically obtained from the full model [colored full lines] and analytically from the reduced model (dashed line) with $M = 6$ meV and taking into account a spacing distance between the two QWs of 6 nm, leading to the estimated value of $\Delta E_1 = 6$ meV, $\alpha = 5$ meV nm (Table 1 in the Appendix). The two situations correspond to the cross and the circle in (a), resp. For $V = 15$ meV, the DQW is topologically non-trivial (b), while for $V = 9$ meV, the system is trivial with no edge states (c).

transition:

$$V_c^2 = \frac{1}{4M^2} \left[ \left( 4M^2 - \frac{\Delta_0^2 + \Delta_2^2}{2} \right)^2 - \frac{(\Delta_0^2 - \Delta_2^2)^2}{4} \right].$$

(9)

This is confirmed by the explicit calculation of the zero invariant $\nu$ with Eq. 3 as shown in Fig. 2 where we calculated the KCN $C_T$, as a function of $\Delta_2$ and $V$. $C_T$ is insensitive to the value of $\alpha$, as long as $\alpha$ and/or $\Delta_2$ remains finite, in which case an insulating gap arises. Interestingly, for $|V| = |V_c|$, lowest bulk bands have at small $k$ a Dirac-like dispersion, while a tunable gap is developed for $|V| < |V_c|$. In the region $|V| < |V_c|$, the system supports an even number of pairs of helical edge modes $N = |C_T|$, in particular $N = 0$ for $M > 0$ and $N = 2$ for $M < 0$. In the outer region, instead, the DQW is topologically non-trivial and allows for a pair of time-reversal protected helical modes. An example of the DQW spectrum in the two regimes, described by Eq. 3 is shown in Fig. 2(b) and (c) (full lines) for a positive mass $M = 6$ meV and a bias of $V = 15$ meV and 9 meV, resp. Edge states are obtained by numerically solving Eq. 3 with open boundary conditions.

In Fig. 2(a) and (b), we plot the wave function of the helical edge states for $E = 0.21$ meV (near the Dirac point) and $E = -1$ meV (near the valence bands), resp. for the system in Fig. 2(b). These states have the peculiarity of supporting at the same time both oscillatory and decaying behavior [clearly evident in Fig. 2(a)], due to the contribution of modes with complex $k_y$, which is related to the Mexican hat shape of the bulk bands. Approaching the bulk bands, the oscillations tend to become less pronounced, as shown in Fig. 3(b). The edge modes have the major contribution from the $H_1$ band of the $f$ layer, which consists in 60% of the probability weight near the conduction band and rises to 90% near the valence band. Under the reversal of $V$, the probability weights of the $b$ and $f$ layer interchange.

III. REDUCED HAMILTONIAN

In order to get an analytical understanding of the system, we derive a reduced 2-band low-energy Hamiltonian $\hat{h}_ll$, with the assumption that the relevant energies are small compared to $\frac{\hbar}{\Delta M} \approx \pm M$. $\hat{h}_ll$ is represented in the basis $\{|E_1, b\}, |H_1, f\}$ or $\{|E_1, f\}, |H_1, b\}$ for the + and − sign, resp. Similar to BLG, we separate the DQW Hamiltonian in Eq. 3 in a low-energy $h_0$ and a high-energy $h_{hh}$ part connected by the off-diagonal blocks $\hat{h}_{hh} = \hat{h}_{hh}$. The reduced 2-band model is obtained then as $\hat{h}_ll = h_0 + h_{hh}G_{hh}h_{hh}$, where $G_{hh} = (E - h_{hh})^{-1}21$. The reduced model $\hat{h}_ll$ can be mapped to a TI Hamiltonian of a single layer (Eq. 1), but with the renormalized parameters

$$\tilde{A} = \frac{\alpha}{2} \pm \frac{A\Delta_\perp}{M \pm \frac{\Delta_0}{2}}, \quad \tilde{M} = \tilde{M} + \frac{V}{2} - \frac{\Delta_0 + \Delta_2^2}{4(M \pm \frac{\Delta_0}{2})},$$

$$\tilde{B} = B - \frac{A^2}{M \pm \frac{\Delta_0}{2}}, \quad \tilde{C} = C - \frac{\Delta_0 \Delta_\perp}{2(M \pm \frac{\Delta_0}{2})}, \quad \tilde{D} = D$$

(10)

while $\tilde{D} = D$ remains unchanged. The bulk dispersion is characterized by a Mexican hat dispersion for $\xi \tilde{M} < \xi \frac{\Delta_0^2}{4\tilde{B}}$, where $\xi = \text{sgn}\left[\tilde{B}(D^2 - \tilde{B}^2)\right]$, with a gap

$$E_g = -\frac{|A|}{\tilde{B}^2} \sqrt{\tilde{A}^2 - 4\tilde{M} \tilde{B}(D^2 - \tilde{B}^2)}.$$ 

If the condition for the existence of the Mexican hat is not fulfilled, the dispersion has a minimum at $k = 0$ and a gap of $2\tilde{M}$. For a barrier thickness of 6 nm, we obtain $E_g \approx -1.6$ meV (see Table 1 in the Appendix for details), which does not strongly depend on $M$. This suggests that the parameters obtained are in the correct ballpark for experiments.

The bulk dispersion curves are quite well reproduced by $\hat{h}_ll$, as demonstrated in Figs. 2(b) and (c) (black dashed lines). However, $\hat{h}_ll$ predicts edge modes with purely linear dispersions $E = -\frac{\tilde{D}}{\tilde{B}} \tilde{M} + s\tilde{A}k_x \sqrt{\tilde{B}^2 - \tilde{D}^2}$, where $s = \pm 1$ denotes the two spin-blocks [colored dashed lines in Figs. 2(b)]. Instead, edge dispersions numerically obtained from the full model [colored full lines in Figs. 2(b)] show a marked non-linear behavior when approaching the bulk bands, with an accompanying shift of the Dirac point.
The Dirac mass parameter $\tilde{\gamma}$ of a single layer of 2D TI. However, the bias voltage enforcing boundary condition at $y = 0$, for the DQW system of Fig. 2(b) near the Dirac point $E \approx 0.21$ meV in (a) and for $E \approx -1$ meV (near the bottom of the valence bands) in (b). In particular, we show the behavior as a function of $y$ of the projection on the $E_1$ and $H_1$ bands of the front (f) and back (b) QWs.

For the reduced model the KCN can be calculated analytically since $F$ assumes the simple form:

$$F_{\mu \nu} = \frac{i}{2} \hat{d} \left( \partial_\mu \hat{d} \times \partial_\nu \hat{d} \right),$$

(11)

where $\hat{d}$ is the unit vector of ($\hat{d}_{x}, -\hat{d}_{y}, \hat{M} - \hat{B}k^2$). The topological features of $H_{11}$ are therefore analogous to those of a single layer of 2D TI. However, the bias voltage enters the Dirac mass parameter $\hat{M}$ thus providing an additional knob to tune a system of two trivial insulators into a single-valley Dirac system ($\hat{M} = 0$) and eventually into a nontrivial TI phase. Since the phase transition at $\hat{M} = 0$ is local at the $\Gamma$-point the analytical topological predictions of the reduced model are inherited by the full model and survive a lattice regularization which makes the KCN mathematically well defined.

Finally, we note that the proposed mechanism of a voltage bias induced band inversion in a DQW is by no means restricted to HgTe based QWs. The method in principle even applies to large band gap semiconductors like GaAs ($V \approx 1$ eV) but the presumably large inversion asymmetry, not captured in our model, would have to be taken into account explicitly.

**IV. DISCUSSION AND CONCLUSION**

It has been proposed earlier that, in single QWs, the topological phase transition may be induced by an effective applied potential[22,24]. In Refs. [22-24], calculations show that in a single Hg$_{1-x}$Cd$_x$Te QW, a potential bias along the well thickness of the order of hundreds of meV [much larger than $V$ needed in our proposal (on the order of a few meV)] induces a band inversion. The experimental feasibility of this approach is arduous due to the large field required. In Ref. [23], a type-II quantum well made of InAs/GaSb/AlSb, which has an intrinsically inverted bandstructure, is considered. The authors show that the spatial separation of $E_1$ and $H_1$ bands offers a key to drive the transition from the TI to the normal phase with an applied gate bias. Recent experiments[25,26] provided the first evidences pointing towards the presence of a TI phase in these kind of structures. The proposal in Ref. [23] requires the growth of a type-II QW, which is a strongly asymmetric structure interfacing two specifically chosen semiconducting materials with different electron affinities (InAs and GaSb). On the contrary, we envision a DQW with each well made from the same material that might be more feasible to experimentally realize clean samples and offers the possibility of tuning the tunneling parameters by modifying the barrier thickness or its chemical composition. This tunability could also be used to create contacts between two helical Luttinger liquids when each QW is in the non-trivial regime and $V \approx 0$. This contact can be either of electrostatic nature which allows to study Coulomb drag[27] or a new type of inter-edge correlated liquid[28], or can induce the tunneling between helical edge states[29].

Further, we note that the LPS ($\vec{P}$) [see Eq. (2)], that operates on the wave function amplitude on the (f) and (b) layers, can be manipulated by the various parameters, in particular by the voltage $V$. As already mentioned, in the regime $V/2 \approx \pm \hat{M}$, the low-energy physics of the DQW is described by Eq. (1), with parameters from Eq. (10), where the basis is given by eigenstates of the LPS with eigenvalues $f$ and $b$ resp. If $\hat{M}$ in Eq. (10) is zero, $\vec{P}$ points in-plane for small in-plane $k$-vector and has a Berry phase of $\pi$ like in graphene. A finite mass $\hat{M}$ tilts $\vec{P}$ out-of-plane and starts to localize $\vec{P}$ in one of the layers. This physics is actually reminiscent of bilayer graphene (BLG) in the presence of an interlayer voltage[28], except that the low-energy physics is governed by a LPS with Berry phase $2\pi$. We expect that interesting proposals that utilize the LPS in BLG, e.g. in a LPS valve[29], also apply here, but with the important absence of a valley degeneracy that is potentially harmful for operating such devices[30]. Also, the application of a voltage domain in BLG predicts valley-filtered edge states at the domain-wall[31] which in our case would result in (Kramers) spin-filtered edge states without valley degeneracy at a mass($\hat{M}$) domain—i.e. helical edge states. Such mass domains would allow the controlled creation of helical edge states not only at the physical sample boundaries of DQW systems but also in their bulk.

In summary, we have investigated DQW structures using the BHZ model of HgTe QWs and a generic tunneling Hamiltonian connecting the layers. An interlayer potential bias on the order of the layer bandgap can drive a
topological phase transition even if the individual QWs are in the normal regime. We calculate the $Z_2$ topological invariant and the helical edge states which in a reduced model obtain simple analytical structures. These results suggest DQWs as potential candidates for an all tunable topological insulator or Dirac system which would have desirable properties for applications.

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Appendix A: Estimate of the tunneling parameters in a HgTe DQW

In the present Appendix, we will provide a quantitative calculation of the tunneling matrix elements [Eq.2] between the electronic states belonging to the front (f) and to the back (b) HgTe/Hg$_{1-x}$Cd$_x$Te quantum wells (QWs) of a double quantum well (DQW) structure. In the first section, we recall the $k \cdot p$ band structure calculations for the confined states of an individual HgTe/Hg$_{1-x}$Cd$_x$Te QW. In the second section, we show how to calculate the tunneling matrix elements arising in a double quantum well configuration, starting from the knowledge of the envelope functions of a single QW and present the numerical values of the single-particle tunneling amplitudes.

1. Band structure model

For the calculation of the band structure and wave functions of the single HgTe/Hg$_{1-x}$Cd$_x$Te QW, an envelope-function approximation$^{23}$, based on an eight-band $k \cdot p$ Hamiltonian, is used. The total wave function is given as follows:

$$\Psi_{k}(r) = e^{i k \cdot r} \sum_{n} f_{n;k}(z) \ u_{n}(r), \quad (A1)$$

where $f_{n;k}(z)$ are the envelope functions, $k = (k_x, k_y)$ is the wave vector in the plane of the QW, and $u_{n}(r)$ is the usual basis set for the eight-band Kane model$^{23}$ which is assumed to be the same in HgTe- and Hg$_{1-x}$Cd$_x$Te layers:

$$u_1(r) \equiv |\Gamma_6, +1/2 \rangle = S \uparrow$$
$$u_2(r) \equiv |\Gamma_6, -1/2 \rangle = S \downarrow$$
$$u_3(r) \equiv |\Gamma_8, +3/2 \rangle = (1/\sqrt{2})(X + iY) \uparrow$$
$$u_4(r) \equiv |\Gamma_8, +1/2 \rangle = (1/\sqrt{6})(X + iY) \downarrow -2Z \uparrow$$
$$u_5(r) \equiv |\Gamma_8, -1/2 \rangle = -(1/\sqrt{6})(X - iY) \uparrow +2Z \downarrow$$
$$u_6(r) \equiv |\Gamma_8, -3/2 \rangle = -(1/\sqrt{2})(X - iY) \downarrow$$
$$u_7(r) \equiv |\Gamma_7, +1/2 \rangle = (1/\sqrt{3})(X + iY) \downarrow +Z \uparrow$$
$$u_8(r) \equiv |\Gamma_7, -1/2 \rangle = (1/\sqrt{3})(X - iY) \uparrow -Z \downarrow. \quad (A2)$$

The Hamiltonian for a QW grown along [001] direction is then given by$^{16}$

![FIG. 4: (Color online) Band edge profile of a HgTe/Hg$_{1-x}$Cd$_x$Te QW of thickness $d$. The profiles of conduction and valence band are shown together with the split-off band (with the split-off parameter $\Delta$).](image)
where

\[
T = E_c(z) + \frac{\hbar^2}{2m_0} (2F + 1)k_z^2 + k_z (2F + 1)k_z, \\
U = E_v(z) - \frac{\hbar^2}{2m_0} \left( \gamma_1 k_z^2 + k_z \gamma_1 k_z \right), \\
V = -\frac{\hbar^2}{2m_0} \left( \gamma_2 k_z^2 - 2k_z \gamma_2 k_z \right), \\
R = -\frac{\hbar^2}{2m_0} \left( \sqrt{3}\mu k_+^2 - \sqrt{3}\gamma k_-^2 \right), \\
S_\pm = -\frac{\hbar^2}{2m_0} \sqrt{3}k_\pm \left( \{\gamma_3, k_z\} + [k, k_z] \right), \\
\tilde{S}_\pm = -\frac{\hbar^2}{2m_0} \sqrt{3}k_\pm \left( \{\gamma_3, k_z\} - \frac{1}{3}[k, k_z] \right), \\
C = \frac{\hbar^2}{m_0} k_- [k, k_z], \\
k_\parallel^2 = k_x^2 + k_y^2, \\
k_\pm = k_x \pm ik_y.
\]

Here, the band structure parameters \(\gamma_1, \gamma_2, \gamma_3, \mu = (\gamma_3 - \gamma_2)/2, \bar{\gamma} = (\gamma_3 + \gamma_2)/2, k\) and \(F\) describe remote band contributions; \(P\) is the Kane momentum matrix element; \(E_c(z)\) and \(E_v(z)\) are the conduction and valence band edges, respectively; \(\Delta\) is the spin-orbit splitting energy. It should be noted, that the in-plane wave vector \((k_x, k_y)\) is a good quantum number, but \(k_z\) should be replaced by the operator \(k_z = -i\partial/\partial z\).

The band structure parameters for HgTe and Hg\(_{1-x}\)Cd\(_x\)Te are considered as piecewise constant for each of the layers with an abrupt change at the interfaces, according to the band edge profile in Fig. 4. Using the correct operator ordering in the Hamiltonian [Eqs. (A3) and (A4)], in accordance with the envelope-function approach derived by Burt\(_{12}\), provides us with an unambiguous determination of the interface boundary conditions. A detailed description of the model, as well as the values of the band structure parameters for HgTe and CdTe, is given in Ref.\(_{16}\).

Solving the eigenvalue problem \(Hf = Ef\) (with \(f\) an eight-component envelope function vector) we determine the envelope functions \(f_{n,k_\parallel}(z)\) and energy levels near \(k_\parallel = 0\) for a single QW. In particular, we are interested in the first conduction and valence subbands which for the QW width close to the critical value 6.3 nm are denoted by E1 and H1.\(_{-}\). Other subbands are sufficiently apart, so that the system can be described, in a reasonable spectral range,\(_{36}\), by a 4-band effective Hamiltonian,\(_{5}\) with the basis given by the E1 and H1 subband eigenstates at \(k_\parallel = 0\) ([E1, +], [E1, −], [H1, +], [H1, −]). Using the eight-band \(k \cdot p\) model described above we calculate these states:

\[
\langle r | E_1, + \rangle = \sum_{n=1,4,7} f_{n,k_\parallel=0}(z) u_n(r), \\
\langle r | E_1, - \rangle = \sum_{n=2,5,8} f_{n,k_\parallel=0}(z) u_n(r), \\
\langle r | H_1, + \rangle = \sum_{n=3,k_\parallel=0} f_{n,k_\parallel=0}(z) u_0(r), \\
\langle r | H_1, - \rangle = \sum_{n=6,k_\parallel=0} f_{n,k_\parallel=0}(z) u_0(r).
\]

The summation index \(n\) usually runs over all eight basis states (see Eq. (A2)). But for \(k_\parallel = 0\) only envelope functions with index \(n\) given in Eqs. (A5) have nonzero

![FIG. 5: (Color online) Envelope functions of the E1 and H1 bands of a HgTe QW of thickness \(d = 5.7\) nm, in panels (a) and (b), respectively, at \(k_\parallel = 0\).](image-url)
values. In Fig. 3a) and (b), we present the envelope functions for E1 and H1 subbands at $k_z = 0$. Note that $f^{E1,+}_{7,k_z=0}(z)$ and $f^{E1,-}_{8,k_z=0}(z)$ give negligibly small contributions to the total wave function $\langle | f^{E1,+}_{7,k_z=0}(z) f^{E1,+}_{8,k_z=0}(z) | \rangle | f^{E1-}_{8,k_z=0}(z) f^{E1-}_{7,k_z=0}(z) | < 0.01$.

2. Tunneling matrix in a double quantum well

We have proposed an extension of the 4-band effective Hamiltonian for a HgTe/Hg$_{1-x}$Cd$_x$Te QW to a DQW structure. Here, we present a realistic estimation of the parameters in the model equation Eq. (2). We consider a DQW geometry as described in Fig. 6 where we assume a symmetric structure for simplicity. Two HgTe QWs of individual thickness $d$ are separated by a barrier of length $t$ of Hg$_{1-x}$Cd$_x$Te. When the barrier is sufficiently thin, the electronic states belonging to different layers share a finite overlap. The envelope function of the DQW can be described as a bonding and antibonding combination of the envelope functions of the individual f and b QWs. Each QW has two confined states in the spectral range of the envelope functions of the individual f and b QWs. The quantitative difference between $\Delta E_1$ and $\Delta E_H$ is strictly a constant. This justifies the treatment of the in-plane wavevector $k_x$ for $t = 7$ nm. Parameter $\Delta E_1$ shows negligibly weak quadratic corrections, while $\alpha$ is strictly a constant. This justifies the treatment of the parameters $\alpha$ and $\Delta E_1$ as constants in Eq. (2).

In Fig. 7(a), we show the dependence of $\Delta E_1$, $\Delta E_H$ and $\alpha k_x$ on the QW separation $t$ for a fixed value of $k_z = 0.1$ nm$^{-1}$ ($k_y = 0$). As expected, both $\Delta E_1$ and $\alpha$ exponentially decay for increasing length of the tunneling barrier. We stress, though, that $\Delta E_H$ is very small and for all practical purposes it can be taken as zero. The qualitative difference between $\Delta E_H$ and $\Delta E_1$ is a direct consequence of the E1 band behaving as an interfacial confined state between HgTe and Hg$_{1-x}$Cd$_x$Te, see Fig. 5. H1 envelope function is, instead, mostly confined in the HgTe layer.

In Fig. 7(b) and (c), we show $\alpha k_x$ and $\Delta E_1$ as a function of the in-plane wavevector $k_x$ for $t = 7$ nm. Parameter $\Delta E_1$ shows negligibly weak quadratic corrections, while $\alpha$ is strictly a constant. This justifies the treatment of the parameters $\alpha$ and $\Delta E_1$ as constants in Eq. (2).

Table I provides the values of $\alpha$ and $\Delta E_1$ for several values of $t$, for a QW of width $d = 5.7$ nm.

Here should be noted that BHZ model is applicable in a finite range of value of the tunneling matrix elements for which the approach we follow is valid. We performed calculations for $d$ in a range between 5.7 nm and 6.6 nm, observing that
the tunneling elements smoothly vary. In particular, for increasing \( d \), \( \Delta_{E1} \) is slightly reduced (there is a variation of about 10% between values corresponding to QW widths of 5.7 nm and 6.6 nm). Parameters \( \alpha \) and \( \Delta_{H1} \) are sensibly increasing with \( d \), however in all the explored range \( \Delta_{E1} >> \Delta_{H1} \).

The DQW geometry, breaking the single QW mirror symmetry, generates also Rashba-like tunneling terms described by Eq. (A7), which are not included in our model for clarity of the presentation. Our calculation shows that the only significant Rashba-like tunneling element is \( \langle E1, +, f | \mathcal{H} | E1, -, b \rangle = \frac{\alpha}{2} k_- \). However, in our proposal there is an energy potential shift \( V \approx \pm 2 M \) between \( f \) and \( b \) QWs. This energy detuning between the \( E1 \) confined levels in the \( f \) and \( b \) QWs strongly hinders their coupling by the Rashba-like interaction. In practice, when we include the Rashba-like term in the model, using the realistic tunneling elements we have calculated, it results in a small (compared to the bandgap) tilting of the bulk dispersion curves (see Fig. 8). Due to this, the dispersion curves are characterized by \( E_{\pm}(k) \neq E_{\pm}(-k) \), with only the time reversal symmetry requirement \( E_{+}(k) = E_{-}(-k) \) still holding. We note that by turning off adiabatically the Rashba-like term, we can connect the system with Rashba-like interactions to that previously presented in the main body of this work without closing the bandgap. This proves that the topological properties of the system are not affected by the Rashba-like tunneling term in Eq. (A7).

In Fig. 8 we show the bulk dispersion curve of a DQW structure employing the tunneling parameters of \( t = 7 \) nm (see Table I), with \( M \approx 6.5 \) meV, corresponding to \( d = 5.7 \) nm, and with a potential shift \( V = -15 \) meV (we note that the electric field employed is about 1 mV/nm, which should be easily achievable in semiconductor heterostructures). Full lines and dashed lines refer to the two Kramer’s blocks. The Rashba-like term in Eq. (A7) is included, with \( \tilde{\alpha} \approx 6 \) meV nm, but its effect, as previously explained, is negligible and consists in a slight tilting of the bands.

A semiconducting gap of 0.85 meV arises, in agreement with the value obtained with the reduced model Eq (10) using the formula

\[
E_g = -\frac{|\tilde{\alpha}|}{B^2} \sqrt{(\tilde{A}^2 - 4\tilde{M}\tilde{B})(D^2 - \tilde{B}^2)}.
\]

Table II shows the value of the bulk gap for several values of \( t \).
For \( t < 5 \) nm, the reduced model (and therefore Eq. [A11]) is no longer valid due to the large tunneling terms \( (H_T) \) compared to the individual QW mass term \( M \), however the full model [Eq.(3)] still holds (as long as the BHZ model is a reasonable approximation of the band structure).

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