Electrical tuning of helical edge states in topological multilayers

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Abstract. A mainstream within topological insulators, GaSb/InAs quantum wells present a broken gap alignment for the energy bands which supports the quantum spin Hall insulator phase and forms an important building block in the search of exotic states of matter. Such quantum wells have electrons and holes confined in different layers, leading to a wide range of possibilities to tune the topological properties. In this work, using a full 3D 8-band $k \cdot p$ method, we study the inverted band structure of GaSb/InAs multilayers under the influence of an electric field applied along the growth direction. By tuning the electric field we change the energy levels of both conduction and valence bands, inducing a topological phase transition in the multilayers. We found that the edge states are predominantly confined in the GaSb layer and that InAs/GaSb/InAs has a large hybridization gap of about 12 meV. Our comprehensive characterization of GaSb/InAs multilayers creates a basis platform upon which further optimization of III-V multilayers can be contrasted with.

\textit{Broken gap, topological, edge states}
We study the electronic band structure for type II broken gap multilayer using a full 3D 8-band $k \cdot p$ method [44, 45] together with the plane wave expansion [49]. In this way, we were capable to have a truncated three dimensional solution of the system which is especially important to analyze the spatial distribution along the confinement profile of the helical edge states' envelope function.

In the inverted band regime the hybridization gap, $\Delta E_h$, is opened at a finite wave vector, $k_c$, with Fermi velocity $v_F \approx \frac{\Delta E_h}{2\hbar k_c}$ [28, 42]. By changing the layer size and/or applying an external electric field, the value of $k_c$ and $\Delta E_h$ can be tuned. Usually, low values of $k_c$ (higher of $v_F$) are desired such that the bulk states do not coexist with the edge states. Hence, a system where $k_c$ is as close as possible to the Γ-point and the $\Delta E_h$ is as large as possible, minimizes all the rich yet undesired physical phenomena [23, 24, 25, 27, 29] that interferes with the edge states. The estimation of the wave vector values in which the hybridization occurs gives the range $k_c \in [0.1, 0.3]$ nm$^{-1}$ suggesting that the systems are in the deeply inverted regime [28]. Moreover, both InAs/GaSb AQWs and GaSb/InAs/GaSb symmetric quantum wells (SQWs) have similar hybridization gap, $\Delta E_h \approx 5$ meV, leading to similar low values of Fermi velocity $v_F \in [1, 4] \times 10^4$ ms$^{-1}$, while InAs/GaSb/InAs SQWs have $v_F \in [3, 9] \times 10^4$ ms$^{-1}$, $\Delta E_h \approx 12$ meV suggesting that InAs/GaSb/InAs SQWs should be a better candidate to host a more isolated Dirac cone.

In summary, the race to build reliable platforms where the properties of the topological phase can be efficiently harnessed is still on. One among several possible applications is to build devices where Majorana fermions could be easily braided [50, 51]. Moreover, very recently it was shown that the hybridization gap of InAs/GaSb/InAs multilayers is temperature independent [52]. Therefore, our study could be used as a guide in order to develop novel devices that use switchable topological phase transitions.
2. Topological Broken-Gap Multilayers

In this manuscript we study two distinct arrangements of broken-gap multilayers that present topological features. The first system, GaSb/InAs/GaSb, consists of one InAs layer surrounded by two GaSb layers, see figure 1(a)-(b), and does not present a hybridization gap. The application of an external electric field induces a Rashba spin-orbit coupling (SOC) that yields a hybridization gap that, as we will show, have values close to the ones of a regular AQW of about 5 meV. In the second system, InAs/GaSb/InAs, consisting of one GaSb layer surrounded by two InAs layers, see figure 1(c)-(d), there is an anticrossing of the electron and heavy-hole (HH) bands but no overall gap (see Supplementary Material). When an electric field is applied the system now shows a hybridization gap of the order of 12 meV that is stable under changes of the applied electric field.

Although the existence of the hybridization gap is important on these systems, its is only effective when this gap results in an overall gap, i.e., that stands for all k points, appearing as a general feature in the DOS of the system. For both configurations we analyze how the hybridization gap changes when Rashba SOC is controlled by the external electric field, directly tuning the values of the overall density of states (DOS) gap. We also analyze the quantum spin Hall phase when we applied the system now shows a hybridization gap of the HH's energy can cross the electron one and the system may be driven from an insulating phase to a band inverted phase \[ \gamma \] \[ \delta \] \[ \epsilon \] \[ \eta \]. In the rest of this article we explore the regimes in which such energy level crossings leads to a topological phase transition by tuning the applied electric field.

2.1. GaSb/InAs/GaSb multilayer

\[ |E| = 1 \text{ mV nm}^{-1} \]
\[ |E| = 3 \text{ mV nm}^{-1} \]
\[ |E| = 5 \text{ mV nm}^{-1} \]

Figure 2. Hybridization gap heatmap of the GaSb/InAs/GaSb SQW as a function of the InAs and GaSb layer sizes. Through (a) to (c) we show the hybridization gaps for several values of external electric field, the star indicate the sizes we use to plot the band structures and projected DOS through (d) to (f), after the band inversion. More specifically, in (a) \( |E| = 1 \text{ mV nm}^{-1} \) \[ \gamma \] \[ \delta \] \[ \epsilon \] \[ \eta \] in (b) \( |E| = 3 \text{ mV nm}^{-1} \) and in (c) \( |E| = 5 \text{ mV nm}^{-1} \). In (d) \( L_{GaSb} = 5 \text{ nm} \) and \( L_{InAs} = 12 \text{ nm} \), in (e) \( L_{GaSb} = 6 \text{ nm} \) and \( L_{InAs} = 10 \text{ nm} \) and in (f) \( L_{GaSb} = 4 \text{ nm} \) and \( L_{InAs} = 12 \text{ nm} \). The wave vector \( k \) in (d), (e) and (f) is defined as \( k = \sqrt{k_x^2 + k_y^2} \).

The energies of the states can be tuned by changing the layer sizes. By changing them it may be possible to align quasi-bond electron states of InAs to quasi-bond hole levels of the GaSb. Thus leading to conditions for resonance tunneling or even giant conductance regime \[ \delta \]. Moreover, as the effective masses of electrons are much smaller than the holes' counterparts, this tuning may be done more effectively by changing the sizes of the InAs layer \( L_{InAs} \).

Carefully adjusting the layers sizes of the GaSb layers \( L_{GaSb} \) the HH'S energy can cross the electron one and the system may be driven from an insulating phase to a band inverted phase \[ \gamma \] \[ \delta \] \[ \epsilon \] \[ \eta \]. In the rest of this article we explore the regimes in which such energy level crossings leads to a topological phase transition by tuning the applied electric field.

Figure 1. Confinement profile of the broken-gap multilayers. (a) and (b) slab configuration with quantum confinement along both y and z directions and quantum well confinement profile for the InAs/GaSb/InAs multilayer system; (c) and (d) slab configuration and quantum well confinement profile for the GaSb/InAs/GaSb multilayer system.
The confinement profile of the GaSb/InAs/GaSb system leads to a spatial separation of the carriers as seen in figure 1(b), electrons being confined in the InAs layer and holes in the GaSb layers. Since there are two identical GaSb layers on both sides of the InAs layer the system presents two important and related features: the valence band states are always (for this range of InAs layer sizes) doubled, leading to a system with inversion symmetry. Without breaking the system inversion symmetry, the GaSb/InAs/GaSb SQW will only have a semiconductor-semimetal transition, as discussed in the Supplementary Material. However, by applying an external electric field we induce the system to change its features: i) the symmetry break gives rise to a Rashba SOC and ii) the potential ramp expels one of the HH subbands from the interacting energy range. The combination of both effects allows the system to have an overall hybridization gap similar to the InAs/GaSb AQWs. As in the SQWs, the Rashba SOC appears only because of the applied electric field, it is fully controllable. By changing the magnitude of the applied electric field along the confinement direction we can only tune the strength of the SOC and, therefore, the magnitude of $\Delta E_h$, but also the $k$ value where band inversion occurs.

Heatmaps showing the overall gap as a function of the $L_{\text{InAs}}$ and $L_{\text{GaSb}}$ are shown in figure 2(a)-(c) for three different absolute values of the electric field $|E| = 1 \text{ mV nm}^{-1}$, $|E| = 3 \text{ mV nm}^{-1}$ and $E = 5 \text{ mV nm}^{-1}$. Two different trends may be extracted from these graphics. First, fixing the size of one layer and of the electric field, if one varies the size of the other layer a threshold is seen in which the hybridization gap opens. Further increasing the size of this layer, the gap reaches a maximum and decays up to a second threshold where the gap closes, forming a crescent moon shape. Second, if the applied electric field value is increased the initial thresholds are moved to a smaller values of $L_{\text{InAs}}$ and $L_{\text{GaSb}}$ and the gaped region is compressed when $L_{\text{InAs}} \approx L_{\text{GaSb}}$ and stretched when they are more separated.

Both behaviors can be explained with a simple argument. The electric field ramp changes the band edges differently for each layer and, consequently, also changes the relative energy difference between states on different layers. For positive (negative) applied electric fields the outer holes states of the left (right) GaSb layer increases in energy while the electron energy level decreases. A trivial band alignment, with electron states having higher energies than holes, may become an inverted alignment for a sufficient large electric field. Further increasing the electric field value may turn this inverted regime system into a deeply inverted regime as in the InAs/GaSb AQW [10] [42].

The deeply inverted regime can be engineered either by finding the right combination of the layer sizes or by an applied electric field. From figure 2(a)-(c) we can identify this regime by choosing a system configuration which is on the verge of becoming gapless. One could also identify it by looking at the wave vector value where the subbands anticross each other, $k_c$. For small magnitudes of the electric field, the hybridization occurs closer to $\Gamma$-point and, therefore, the value of $k_c$ is also smaller, compared to large values of electric field in the same system. In our data, the values vary in the ranges of $k_c \in [0.1, 0.3] \text{ nm}^{-1}$ and $v_F \in [1, 4] \times 10^4 \text{ m s}^{-1}$ and though, GaSb/InAs/GaSb SQW shows a deep hybridization.

Figure 2(d)-(f) present the band structures and the projected DOSs for selected deeply inverted regime SQWs, marked as a star in figure 2(a)-(c), respectively. The band structures were plotted as functions of all $k$ setting $k = \sqrt{k_x^2 + k_y^2}$ allowing the visualization of features from all directions of the band structures at once. The asymmetries of the valence band become very clear for wave vectors away from $\Gamma$-point, showed as the spreading in energy of a given subband. In the inverted regime the largest contribution in the projected DOS near the hybridization gap region are due to the HH band. Although the conduction band state should be a linear combination of electrons and light-holes, as explicitly shown in simplified models of topologically protected systems, like the Bernevig-Hughes-Zhang (BHZ) model [56], the light-hole contribution is only relevant for wave vectors away from the $\Gamma$-point and/or energies well bellow the hybridization region. This means that in order to correctly describe the low-energy spectrum of such SQW there is no need to include the a light-hole band, as it is important for the InAs/GaSb AQW [42] [6], although we need to include the extra HH band [7].

The effect of the electric field in expelling the lower HH subbands can be seen in figure 2(d), 2(e) and 2(f). In figure 2(d) both HH subbands are almost degenerate at $\Gamma$ with energies close to 0.31 meV. The spin-splitting of each subband is seen at higher $k$ [1]. In figure 2(e), the second HH appears at around 0.25 meV and in figure 2(f) it is out of the range. Therefore, in the limit of very large electric fields the system becomes similar to the InAs/GaSb AQW, i.e., the electric field isolates one of the GaSb layers from the GaSb/InAs and simpler models such as the aforementioned BHZ model [56] can describe very accurately the low energy properties of the system.

Massless Dirac fermions The investigation of the Dirac cones and edge states are usually done by using effective models that include a limited number of bands, such as the 4-band BHZ model [56] and...
Figure 3. Energy dispersion and edge states probability densities for a $L_{GaSb} = 5$ nm and $L_{InAs} = 12$ nm SQW. (a)-(e) are for $E = 0$. (f)-(j) are for $|E| = 1$ mV nm$^{-1}$. (k)-(o) are for $|E| = 5$ mV nm$^{-1}$. The colors in the probability densities represent the localization of the states. The green line in (a) is a guideline to highlight where the Dirac cone is.

other extended BHZ-like models that include extra subbands [6, 7]. The advantage of these models is the number of states included, requiring smaller computational resources to be numerically solved. What makes them simpler, in few words, is that symmetry is used to define a basis, with a smaller number of states that describes the essential features of the system in the confinement direction, the quantum well growth direction. This basis is composed by states that are linear combinations of components of the original basis specific tuned to describe the intended few subbands near the gap. Then this direction, the $z$, is integrated out and replaced by a set of parameters. The integration that allows to simplify the description is also its major drawback, since the spatial resolution along $z$ of the probability densities along the quantum well confinement is lost. Here, instead of using the BHZ-like models, we use the full 3D 8-band $k \cdot p$ model, and therefore, we kept the spatial resolution along the quantum well confinement axis.

Analyzing the system without the application of an electric field, although it does not present the hybridization gap, one of the HH subbands is hybridized with the electron subband. By confining the multilayer along one of its free direction we see, in figure 3(a), that the system has a linear energy dispersion band (emphasized by the green line), but it is embedded on the valence subbands, i. e., there is an edge state that connects the conduction band to the second valence band [7].

To verify that indeed this embedded linear energy dispersion corresponds to edge states, we plot in figure 3(b)-(e) the probability density of such states, for the conduction band (upper panels) and valence band (lower panels) at $k_y = 0.026$ nm$^{-1}$ ((b) and (c)) and at at $k_y = 0.077$ nm$^{-1}$ ((d) and (e)). Notice first, that each state is doubly degenerate in spin. Therefore, in figure 3(b) and 3(c) we plot the probability density of one of the spin components, while in figure 3(d) and 3(e) we plot the other spin component, for a given wave vector. It is evidently clear that these states are helical edge states since each spin projection is confined along an opposite edge of the slab. A distinctive feature of these edge states is that they are oscillating, i. e., they have peaks and nodes along the $y$ direction, but in general the density present a very intense peak near the edge and the intensity of the peaks toward the center diminish, forming a tail. Moreover, by using the full 3D $k \cdot p$ description we are able to see that the edge states are symmetric with respect to the InAs layer (central layer) and are predominantly located into the GaSb layers, although for $k_y = 0.077$ nm$^{-1}$ the conduction band edge state is still predominantly in the GaSb layers, it is also more spread throughout the slab and does not present oscillations indicating that it is losing its edge state character and is becoming a bulk like state. Nevertheless, for the same wave vector, the valence band edge state is still mostly at the edge.
In order to isolate the Dirac cone we applied an electric field to generate a Rashba SOC and also to push one of the HH bands away. In figure 3(f)-(j) we show the energy dispersion and the probability densities for the same GaSb/InAs/GaSb multilayer with applied electric field of $|E| = 1 \text{ mV nm}^{-1}$. In figure 3(f) we see that indeed the second HH band is not anymore on the same energy range as the Dirac cone and that it has become very visible and well isolated from the other subbands. The probability densities are shown on figure 3(g)-(j), but now at four distinct wave vector values and its worth noticing that, although we are only showing one of the spin components, they have peaks at both interfaces with opposite spin projections (as it should be for helical edge states) [57]. Since there is an applied electric field, the states are not anymore symmetric with respect to the InAs layer, however they still are predominantly confined on the GaSb layers. The probability densities at $k_y = 0.026 \text{ nm}^{-1}$ and $k_y = 0.077 \text{ nm}^{-1}$ show the edge states with oscillation and light tails as seen in figure 3(g) and 3(h). As the wave vector increases however, the overall behavior of these oscillations change and the more intense peaks start spreading from the edges to the center of the slabs, as seen in the valence band panel of figure 3(h). Further increasing the wave vector, the oscillations end on the conduction band, even though the state still has a higher confinement on the GaSb layer – but persists on the valence band but now the oscillations are in small number and more intense at the center of the confining potential, as seen in figure 3(i). This mixed state is on the transition from an edge state to a bulk state and we can see that its wave vector is at the point where the Dirac cone dispersion touches the bulk-like energy dispersion. Choosing the wave vector away from the Dirac cone region, see figure 3(j), the states indeed become bulk-like states in which the conduction band edge state remains very well confined on the GaSb layer.

A striking feature of some quantum spin Hall systems, such as InAs/GaSb AQW and HgTe/(Hg,Cd)Te QWs is that it was experimentally observed that they host a robust helical edge state which persists up to several Tesla. This robustness was latter on explained by the burying of the Dirac cone into the valence subbands [0, 5]. Here, we also show that proposed SQW quantum spin Hall system also has such buried Dirac cone, and therefore hosts a robust edge that should persists up to several Tesla. In general, for such feature to be presented in the SQW they have to be in the deeply inverted regime. Therefore if a selected system does not present the buried Dirac cone, a recipe to achieve it is to increase the applied electric field, thus enhancing the inverted regime. In figure 3(k) we can see that by increasing the applied electric field we push the subband crossing point away from the Γ-point (it is at 0.0 nm$^{-1}$ in (a), a little below 1.28 nm$^{-1}$ in (f) and close to 0.2 nm$^{-1}$ in (k)), meaning that (k) is on a deep inverted regime. Focusing on the right panel of figure 3(k) one can see that, indeed, the Dirac cone was pushed down towards the bulk valence subbands and it is hidden.

In figure 3(l)-(o) we show the probability densities of four selected wave vector values. For a wave vector near Γ-point the edge states are very confined at the edges, with oscillations and a light tail towards the middle of the confinement profile, as seen in figure 3(l). As we increase the wave vector, the oscillations of the valence band edge state are accentuated, but the conduction band edge state remains very well confined to the edge, as seen in figure 3(m). In figure 3(n) and 3(o) the wave vectors are near the $k_c$ value, i.e., the crossing point between the conduction and valence subbands, and therefore one should expect that the probability densities become more similar to a bulk state than to an edge state. Indeed, this is what happens for the valence band edge state, although it has a highly oscillating pattern while the conduction band edge state remains well confined at the edge.

In summary, the hybridization gap for the GaSb/InAs/GaSb SQW have a similar magnitude as the InAs/GaSb AQW. The presence of an extra HH subband, due to the second GaSb layer, precludes the opening of the hybridization gap and the system only has a semiconductor-semimetal transition. The application of an external electric field is therefore a requirement to open the hybridization gap. Moreover, estimation of $k_c$ and $v_F$ indicate that this system is in a deeply inverted regime. By confining along the $y$ direction and analyzing the spatial distribution of the edge states we discovered that they are predominantly confined at the GaSb layer. As we could see, in figure 3 as we increase the applied electric field and enhance the inverted regime, the probability densities become more oscillating and its overall maximum go further to the middle of the confining profile.

### 2.2. InAs/GaSb/InAs multilayer

In the InAs/GaSb/InAs configuration, electrons are confined in the lateral wells and the holes inside the central well. The tuning of the layer sizes may be used to transition from a trivial to a band inverted regime. Differently from the GaSb/InAs/GaSb case, the hybridization gap is always present, but the system does not show an overall gap in the absence of an external electrical field. As shown in the Supplementary Material, the semiconductor-semimetal transition occurs as a result of the interaction of the subbands that gradually shifts the top of the valence
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In this section we will investigate the Dirac cone and edge states of the InAs/GaSb/InAs using the full 3D 8-band \( \mathbf{k} \cdot \mathbf{p} \) model. In the inverted regime with the addition of an applied electric field, the hybridization gap is always present and by confining the system along one of its free directions it shows a very clear linear energy dispersion \[7\], as seen in figure \(5\) (a).

Figure \(5\) (b)-(e) present the probability densities of the edge states at four selected wave vector values. Notice that contrary to the previous case, the linear dispersion here is not embedded on the valence subbands and instead it is isolated at the hybridization gap energy region. Only one of the spin components of each state is shown since the other component is its conjugate.

For \( k_y = 0.026 \text{nm}^{-1} \), the edge states are well confined at the edges of the system and the oscillatory tail towards the middle of the slab have almost zero intensity, as seen in figure \(5\) (b). Moving away, for \( k_y = 0.077 \text{nm}^{-1} \) (figure \(5\) (c)), the conduction band states have already become bulk-like states with the...
The application of an external electric field accentuates the edge states features. From the previous section we know that it pushes the second electron subband away from the hybridization energy range and the $k_z$ is pushed further away from the Γ-point. Figure 5(g)-(j) show probability densities for selected wave functions in a system with $|E| = 1$ meV/nm. For $k_y = 0.026$ nm$^{-1}$, the edge states are very confined at the edges with almost no oscillatory tail towards the center of the slab, as seen in figure 5(g). Figure 5(h) shows that both, conduction and valence band states at $k_y = 0.077$ nm$^{-1}$, are still edge states. However, the conduction band density probability has a non-oscillatory stronger tail towards the center of the slab and both states are more localized in the GaSb region. Moving to $k_y = 0.128$ nm$^{-1}$ and $k_y = 0.179$ nm$^{-1}$, we get away from the Dirac cone region and, indeed, the states becomes bulk-like and conduction band states become localized at one of the InAs regions, as seen in figure 5(i) and 5(j).

The estimations of the Fermi velocities for the InAs/GaSb/InAs QW, $v_F \in [3, 9] \times 10^4$ m/s, indicates that it should not be in an as deeply inverted regime than its counterpart GaSb/InAs/GaSb SQW. Indeed, by analyzing the probability densities of both QWs we gather that the former has well localized edge states while the latter has edge states with a highly oscillating tail. Moreover, by decreasing the hybridization gap, $\Delta E_h$, the Fermi velocity also decreases and the system move towards a more inverted regime. In such a situation we should see edge states with an oscillatory tail as it was shown before.

By increasing the applied electric field we can tune the system to a deeply inverted regime, as discussed before, where the Dirac cone becomes buried in the bulk valence subbands. In figure 5(k) we present the energy dispersion showing a distinct case since the top of the valence band is at a finite wave vector away from the Dirac cone is hidden. Focusing on the right panel of figure 5(k) one indeed see that the Dirac cone is hidden.

Figure 5(l)-(o) show the probability densities of four selected wave vector values. For $k_y = 0.026$ nm$^{-1}$ the edge states are very confined at the edges with a slightly oscillating tail, as seen in figure 5(l). As the wave vector increases, the oscillations of the conduction
band edge state are accentuated, but the valence band edge state remains unchanged, as seen in figure 5(n). In figure 5(n), for \( k_y = 0.128 \text{nm}^{-1} \), the conduction band edge state has switched to a more bulk-like state with a higher probability to be found in the center but still with an oscillating pattern, while the valence band is still well localized at the edge. Moving to \( k_y = 0.179 \text{nm}^{-1} \), see 5(o), we are still inside the hybridization region, although both conduction and valence states had acquired a more bulk like shape they are not yet fully bulk states.

In summary, the hybridization gap for the InAs/GaSb/InAs SQW is about 12 meV and larger than both GaSb/InAs/GaSb SQW and InAs/GaSb AQW. Moreover, estimation of \( k_c \) and \( v_F \) indicates that the system is not so inverted as its counterparts. By confining along the \( y \) direction and analyzing the spatial distribution of the edge states also verifies that they are predominantly confined at the GaSb layer. As we could see, in figure 5 the edge states are very localized at the edges with very small oscillating tail, if any. By increasing the electric field we could transition the system to a deeply inverted one with a hidden Dirac cone.

3. Modeling details

To correctly account for the hybridization of the conduction and valence bands an accurate description of the valence band states is needed, specially for the heavy- and light-hole states. The usual 8-band Kane model \([45]\) is not adequate for this description since it gives the wrong value for the effective mass of the HH states in certain materials \([53]\). In this work we used the 8-band \( \mathbf{k} \cdot \mathbf{p} \) model including the conduction band states, the three valence bands, the explicit coupling between them and the Luttinger corrections for the effective masses. \([44, 46, 47]\) This model has been successfully applied in describing the electronic and spintronic properties of low dimensional semiconductor for decades \([59, 60, 61, 62, 63, 64]\), including the InAs/GaSb AQWs. \([6, 5, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74]\)

The \( \mathbf{k} \cdot \mathbf{p} \) model describes a bulk material around a high symmetry point, usually the \( \Gamma \)-point, where the physics of interest takes place. To correctly describe it, a parametrization of the matrix elements among the basis states (Bloch functions) is derived using Group Theoretical methods. To describe a heterostructure, as a QW, we apply the envelope function approximation \([48, 58]\), that defines the total wave function of a state of the system as a continuous and slowly varying function, called the envelope function, that is weighted by the Bloch’s function of each material. The quantum confinement along the growth direction essentially means that we have to make the substitution \( k_z \rightarrow -i \frac{\partial}{\partial z} \). This approach results in a system of coupled linear differential equations. This system is solved by applying the plane wave expansion, using the Fourier transformations– using 40 planes waves which suffices to achieve energy convergence in our calculations. The method is well described in our previous works \([60, 64]\). We solve the final matrix Hamiltonian by direct diagonalization methods using the MAGMA \([75]\) suite which implements the LAPACK routines in a multicore + GPU (graphical processing unit) computational environment.

The parameters used in the 8-band \( \mathbf{k} \cdot \mathbf{p} \) model were extracted from Ref. \([76]\). It is know that solution of narrow gap semiconductors is plagued with spurious solutions and to avoid it we apply a renormalization of the Kane interband momentum matrix element, \( P \), as suggested by Ref. \([77]\).

\[
P^2 = \left( \frac{m_0}{m_c} - 1 \right) \frac{E_g (E_g + \Delta)}{E_g + \frac{2}{3} \Delta} \frac{\hbar^2}{2m_0}
\]

where we set \( \frac{m_0}{m_c} = 1 \) with \( E_g \) being the gap energy and \( \Delta \) the spin-orbit splitting energy. With the new \( P \) we then calculate the new corrected Luttinger parameters according to

\[
\begin{align*}
\gamma_1 &= \gamma_1 - \frac{E_p}{3E_g} \\
\gamma_2 &= \gamma_2 - \frac{E_p}{6E_g} \\
\gamma_3 &= \gamma_3 - \frac{E_p}{6E_g} \\
A &= \frac{1}{m_e^*} - \left( \frac{E_g + \frac{2}{3} \Delta_{SO}}{E_g + \Delta_{SO}} \right) \frac{E_p}{E_g}
\end{align*}
\]

4. Conclusion

In this manuscript we have explored the electric control of the topological phase transition in GaSb/InAs/GaSb and InAs/GaSb/InAs symmetric multilayers and the spatial distribution of the edge states probability density using a full 3D 8-band \( \mathbf{k} \cdot \mathbf{p} \) method.

We have shown that the hybridization gap for the GaSb/InAs/GaSb SQW have values around 5 meV that are very similar to the InAs/GaSb AQW, while for InAs/GaSb/InAs SQW is about 12 meV. In both systems the hybridization occurs at similar values of wave vector \( k_c \in [0.1, 0.3] \text{nm}^{-1} \), therefore the InAs/GaSb/InAs SQW having a large hybridization gap will also have a larger Fermi velocity. Ultimately, this means that the edge states of the InAs/GaSb/InAs SQW are less interacting with the bulk bands.
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By applying a weak confinement along the $y$ direction and analyzing the spatial distribution of the edge states we verified that they are predominantly confined at the GaSb layer. By increasing the electric field we tune the system to a deeply inverted regime with a hidden/buried Dirac cone having highly oscillating probability densities with large tails towards the bulk. Although this feature is present in both multilayers, the InAs/GaSb/InAs SQW due to its large hybridization gap, suppress it, and therefore is suggested as the better option to explore the rich physics offered by the quantum spin Hall.

Combining the facts i) that superconductivity has been induced in the InAs/GaSb edge states [26] and, ii) that braiding of Majorana fermions is theoretically achievable using magnetic textures from commercially available magnets [50, 51] and, iii) that the hybridization gap of InAs/GaSb/InAs multilayers is temperature independent [52] with our realistic calculations showing that indeed InAs/GaSb/InAs shows topologically protected edge states, we suggest that these multilayers can be a very plausible alternative for the future of fault-tolerant quantum computing devices.

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