An all electron topological insulator in InAs double wells

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We show that electrons in ordinary III-V semiconductor double wells with an in-plane modulating periodic potential and inter well spin-orbit interaction are tunable Topological Insulators (TIs). Here the essential TI ingredients, namely, band inversion and the opening of an overall bulk gap in the spectrum arise, respectively, from (i) the combined effect of the double well even-odd state splitting $\Delta_{\text{SAS}}$ together with the superlattice potential and (ii) the interband Rashba spin-orbit coupling $\eta$. We corroborate our exact diagonalization results by an analytical nearly-free electron description that allows us to derive an effective Bernevig-Hughes-Zhang (BHZ) model. Interestingly, the gate-tunable $\Delta_{\text{SAS}}$ drives a topological phase transition featuring a discontinuous Chern number at $\Delta_{\text{SAS}} \sim 5.4$ meV. Finally, we explicitly verify the bulk-edge correspondence by considering a strip configuration and determining not only the bulk bands in the non-topological and topological phases but also the edge states and their Dirac-like spectrum in the topological phase. The edge electronic densities exhibit peculiar spatial oscillations as they decay away into the bulk. For concreteness, we present our results for InAs-based wells with realistic parameters.

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Topological Insulators have been theoretically predicted in graphene \cite{1} and in negative-gap or inverted-band HgTe-based quantum wells \cite{2}, being experimentally realized in the latter shortly after \cite{3}. These are exotic solids being bulk insulators with metallic edges or surfaces \cite{4,5}. An essential ingredient for a system to exhibit topological insulating phases is the existence of a tunable bulk band gap that can not only be tuned to zero but also invert its sign. Defining as “positive gap” the case in which it can be mapped without closing onto the $m_0c^2 > 0$ gap separating the positive- and negative-energy solutions of the Dirac equation (“vacuum”), one can immediately see that an interface between materials with positive and negative gaps must support gapless (edge or surface) states \cite{6}. Time reversal symmetry and spin orbit interaction inextricably lock the spin and momentum of these states making them helical \cite{7}.

More recently, interesting works have proposed TIs with ordinary bulk materials \cite{8,9,11}, as naturally occurring inverted-band or negative-gap materials are usually unconventional narrow band-gap systems. These proposals rely on externally inducing a band inversion of the electron and hole states, e.g., electrically in double well systems \cite{8,9,12}. Hexagonal patterns fabricated in p-doped GaAs well to resemble the physics of Dirac carriers in graphene offer yet another means to attain topological insulating phases \cite{10}. Yet another appealing idea is the use of built-in polarization fields to induce band inversion and TI phases in Ge sandwiched between GaAs layers \cite{11}. All of these works rely on electrons and holes \cite{8,9,11} or holes only \cite{10}.

Here we propose a TI based on ordinary III-V semiconductor nanostructures with only electrons. We consider a bilayer quantum well with two confined electron subbands and intersubband spin-orbit coupling \cite{13,14}. Fig. 1a. Upon modulating the well potential to make a superlattice within the plane of the well via properly defined metallic gates, or etching, on top of the two dimensional electron gas, Fig. 1b, we are able to obtain the necessary ingredients for a TI \cite{15}: (i) tunable inverted subbands controlled by the ‘mass’ parameter $2M = \Delta_{\text{SAS}} - \Delta_V$ that depends on both the (gate-controllable) double-well even-odd state splitting $\Delta_{\text{SAS}}$ and the parameter $\Delta_V$ that is determined by the form of the periodic potential and (ii) a bulk overall gap controlled via the interband spin-orbit coupling $\eta$ that gives rise to anti crossings, see bands around the $\Gamma$-point in Fig. 2. In principle the Fermi energy can be tuned so as to lie in the bulk gap.

We first solve the problem within the physically appealing nearly-free electron description. In this approach...
we analytically derive an effective BHZ model for our system 2. We also solve the problem numerically via exact diagonalization thus determining the full energy spectrum within the Brillouin zone. In the appropriate parameter range the two descriptions agree very well. We also calculate the topological invariant (Chern number) from our bulk band structure and show that the system undergoes a topological phase transition driven by the gate-tunable interlayer coupling $\Delta_{\text{SAS}}$. The Chern number shows a discontinuity at $\Delta_{\text{SAS}} \approx 5.4$ meV where $M = 0$. We then find the solutions for a strip configuration to verify the bulk-edge correspondence explicitly: in the non-topological phase ($\Delta_{\text{SAS}} > 4.5$, $M = 0$) our system is a bulk insulator with no edge states while in the topological regime ($\Delta_{\text{SAS}} < 5.4$, $M < 0$) it features, in addition, gapless edge states with Dirac-like bands. Interestingly, we find that the edge states display oscillations as they spatially decay away from the border into bulk. These oscillations can in principle be mapped via scanning gate microscopy recently used to probe edge states in HgTe-based TI wells 7.

Model system. Our effective $4 \times 4$ model describes the two lowest subbands of a symmetric quantum well (plus spin). In the basis of the (e)ven and (o)dd eigenstates $\{|p, e \uparrow\rangle, |p, o \downarrow\rangle, |p, e \downarrow\rangle, |p, o \uparrow\rangle\}$ we have

$$H_w(p) = \begin{pmatrix} \frac{p^2}{2m^*} & \eta p - i \frac{\pi}{2p} & 0 & 0 \\ 0 & 0 & \frac{p^2}{2m^*} & -i \frac{\pi}{2p} \\ 0 & 0 & 0 & \frac{p^2}{2m^*} + \Delta_{\text{SAS}} \\ 0 & 0 & -i \frac{\pi}{2p} & \frac{p^2}{2m^*} + \Delta_{\text{SAS}} \end{pmatrix}$$

(1)

where $p$ denotes the electron’s momentum and $p_\pm = p_x \pm i p_y$. Here $\eta$ is the interband spin-orbit coupling 13 and $m^*$ the electron effective mass. The Hamiltonian in (1) can be put into the standard BHZ form by the unitary transformation $U = e^{-\sigma_3 \pi p/4}$ acting on each $2 \times 2$ diagonal block. This results in the new $2 \times 2$ upper diagonal block

$$H_{w,2 \times 2}(p) = \begin{pmatrix} \frac{p^2}{2m^*} + \Delta_{\text{SAS}} & \eta p \pm i \frac{\pi}{2p} \\ \eta p \mp i \frac{\pi}{2p} & \frac{p^2}{2m^*} + \Delta_{\text{SAS}} \end{pmatrix}.$$ \hspace{1cm} (2)

The lower diagonal block is the time reversed version of Eq. (2): $H_{w,2 \times 2}^*(-p)$. Equation (2) has a form reminiscent of the $2 \times 2$ diagonal blocks of the BHZ model, apart from the inverted band structure 2. In the BHZ model the inverted band structure arises from the peculiar ordering of bands of HgTe combined with the tunability of the electron and hole levels in a well geometry. Here we will engineer an inverted-band system from the ordinary double well with normal ordering of bands by superimposing a two dimensional superlattice on top of it, Fig. 4b. We choose the periodic potential (period $L$) as

$$V(r) = V_1 \cos(Qx) + \cos(Qy) + V_2 \cos(Qx) \cos(Qy),$$ \hspace{1cm} (3)

where $Q = \frac{2\pi}{L}$. Equation (3) is plotted in Fig. 4b) for $V_1 = 3.5$ meV, $V_2 = 12.0$ meV. This potential gives rise to parabolic dispersions around the $\Gamma$-point with positive curvature (mass) for the lowest band and negative curvature for the third band, thus leading to the relevant inverted bands needed. More specifically, the superlattice Hamiltonian is

$$H_{\text{SL}} = H_{w,2 \times 2}(-ih\partial_x, -ih\partial_y) + V(x, y)I_{2 \times 2}.$$ \hspace{1cm} (4)

where we have used $p = -ih\nabla$. The corresponding eigensolutions are Bloch wave functions $\psi_{k,n}(r) = e^{iK \cdot r} u_{k,n}(r)$ with energies $\varepsilon_n(k)$, $u_{k,n}(r)$ has the same periodicity as $V(r)$. From now on $k$ denotes the wave vector characterizing the superlattice energy bands.

It is convenient to define the energy scale $E_Q = \frac{\hbar^2 Q^2}{2m^*}$, which for InAs ($m^* = 0.222$) and, say, $L = 80$ nm, yields $E_Q \approx 10$ meV.

Gapped bulk spectrum. Figure 2 shows the band structure (red curves 17) obtained via exact diagonalization using the parameters: $V_1 = 3.5$ meV, $V_2 = 12.0$ meV, $\Delta_{\text{SAS}} = 4.5$ meV, and $\eta = 20$ meVnm 13. The interband coupling $\eta$ can be further increased by optimizing the quantum well structure 13. The $V_2$ term opens up a gap at the $\Gamma$-point, giving rise to a negative curvature band, and $V_1$ facilitates the coupling between the second and third states for finite $k$ values, see Eqs. (5) and (6). When $V_2 \approx E_Q$ the gap opens up over the full Brillouin zone. The gray dashed curves shows the bands in the absence of the spin-orbit coupling $\eta$. The 2nd and 3rd bands clearly show inversion and crossings for $\eta = 0$, while a non-zero $\eta$ opens up gaps at the crossing (red curves). The energy splitting of the inverted bands is given by $2M = \Delta_{\text{SAS}} - \Delta_V$. The parameter $\Delta_V$ is de-
defined as the energy difference between the 1st and 3rd energy bands at the Γ-point [19], see Fig. 2. The value of the even-odd energy splitting $\Delta_{SAS}$ is controlled by the structure of the quantum well confining potential. The inset in Fig. 2 is a blowup of the band crossing for $\Delta_V = 5.4$ meV and three different values of $\Delta_{SAS}$, going from an inverted ordering of bands for $M = -0.45$ meV and $-0.2$ meV to a normal ordering at $M = 0.1$ meV.

**Nearly-free electron description.** Here we focus on the 2nd and 3rd bands for $\eta = 0$ (see gray curves in Fig. 2), which comprise the two inverted crossing bands required by the BHZ model. To obtain analytical results and a better understanding of our system we now follow a perturbative approach even though our periodic potential strength is comparable to $E_Q$. By doing lowest order perturbation theory in $V$, we focus on the free-electron bands at the Γ-point. We now use the $M^2$-vector of the BHZ model [2] given by

$$\begin{align*}
d_{x,y}(k) & = i\eta \int d^2 r u_{k,3}^*(r) \partial_{x,y} u_{k,2}(r) \\
& \approx \eta \sqrt{2V_1 \frac{V_2}{V_1}} k,_{x,y},
\end{align*}$$

where we have used Eqs. (5) and (6) and further assumed $V_2 \gg V_1, \frac{\hbar^2 k^2}{2m}$ for simplicity. The component $d_z(k)$ is given by the energy difference between bands 2 and 3

$$d_z(k) = \frac{1}{2}(\varepsilon_3(k) - \varepsilon_2(k)).$$

In Fig. 3a) we plot $d_z(k)/|d(k)|$ (color plot) and $d_x(k),d_y(k)$ (arrows) using the exact solutions for the states 2 and 3.

**Topological index.** From the $d$-vector [Eqs. (7) and (9)] we calculate numerically the topological invariant

$$C_1 = \frac{1}{4\pi} \int d^2 k d(k) \cdot (\partial_1 d(k) \times \partial_2 d(k)); \ d = \frac{d}{|d|}$$

for distinct $\Delta_{SAS}$’s around the critical value $\Delta_{SAS} \approx 5.4$ meV. As can be seen in Fig. 3b) the invariant jumps by one when the $\Delta_{SAS}$ crosses 5.4 meV, thus signaling that the system undergoes a transition from a topological-insulating phase to a trivial insulating phase.

**Strip configuration: edge states.** Here we verify the bulk-edge correspondence by explicitly finding the edge states of the system in a finite geometry for both the topological and non-topological phases. We solve the Hamiltonian in Eq. (1) for a strip of width $L_x$, using open boundary conditions (‘hard wall’) $\psi(0,y) = \psi(L_x, y) = 0$. Bloch’s theorem still applies in the longitudinal direction. We expand the transverse part of the wavefunction in a normalized sine basis. The number of transverse states is truncated at $N_{\text{per}} = 5 N_{\text{max}}$ where $N_{\text{per}}$ is the number of periods of the potential that fit into $L_x$. This corresponds to including, roughly, 5 $Q$-vectors in the $y$-direction in the bulk model. Solving Eq. (4) for a given value of $k_y$ yields $2 \times 5 N_{\text{per}}$ eigenvalues. Focusing on the eigenvalues in the energy interval corresponding to the BHZ bands, one can plot the relevant set of eigenvalues as function of $k_y$.

In Fig. 4a) the value of $\Delta_{SAS} = 4.5$ meV corresponds to the topological phase (see inset in Fig. 2) and indeed we see edge states in the gap. In Fig. 4b) the even-odd splitting is increased to $\Delta_{SAS} = 5.6$ meV and the edge states are absent, since the system has now turned to a normal insulator. As can be seen in Fig. 2b) $\Delta_{SAS}$ controls the magnitude and the sign of the gap. Using the BHZ notation, the edge state in Fig. 4a) corresponds to a negative gap $M = d_x(0) < 0$, Fig. 4b) where $M$ is positive and no gap states appear. Note that for $\Delta_{SAS} = 4.5$ meV our system can not be approximated by an effective BHZ model as the bands show substantial non-parabolicity. This does not influence the existence of the edge states in our system.
Oscillatory decaying edges. In order to compare our results to the known analytical solution of the BHZ model, we focus on $\Delta_{SAS} = 5.2$ meV, for which the parabolic approximation is better. We can extract the BHZ parameters directly by fitting the curves appearing in the inset of Fig. 2 to the eigenstates of the BHZ model, i.e. Eq. (5) in Ref. [5]. From these values we can calculate the properties of the edge states using the ansatz $\psi(x) \propto e^{i\lambda x}$ and $E = -DM/B$, solving for $\lambda$ in the middle of the gap ($k_y = 0$ and $E = -DM/B$) results in

$$\lambda = \pm \left( \frac{A}{2\sqrt{B^2 - D^2}} \pm i \sqrt{\frac{M}{B} - \frac{A^2}{4(B^2 - D^2)}} \right). \quad (11)$$

Note that for the parameters extracted from the bulk spectrum $\frac{M}{B} - \frac{A^2}{4(B^2 - D^2)} > 0$, which yields a $\lambda$ with a non-zero imaginary part in addition to a real part. This gives rise to a localized edge state that oscillate spatially. Indeed we see from the numerical diagonalization of Eq. (1) that the edge state decays into the bulk with slower oscillations due to the imaginary part of $\lambda$ and rapid oscillations due to the period of the superlattice. The probability densities of the edge states corresponding to $\Delta_{SAS} = 5.2$ meV for strip widths $L_x = 40L$ and $L_x = 80L$ are shown in Figs. 3a) and b), respectively. For $\Delta_{SAS} = 5.2$ meV the decay length and oscillation wavelength are where $1/\mathrm{Re}(\lambda) = 11.5L$ and $\frac{2\pi}{\mathrm{Im}(\lambda)} = 11.8L$, respectively [21]. For a given energy in the gap there are two edge states localized at opposite edges, $\psi_{+k_y}^{+}(x)$ localized around $x = 0$ and $\psi_{-k_y}^{-}(x)$ localized around $x = L_x/2$. The density of the BHZ edge state localized around $x = 0$, using parameters extracted from Fig. 2 and $k_y = 0$,

$$|\psi_{BHZ}(x)|^2 \propto \exp(-2x\mathrm{Re}(\lambda)) \sin^2(\mathrm{Im}(\lambda)x), \quad (12)$$

agrees well with the numerical results (blue curves in Fig. 5). Note that the edge state density is symmetric for $k_y = 0$ [20]. The helical character of the edge-states comes from the time reversed part of the $4 \times 4$ hamiltonian, see discussion below Eq. (3). In Fig. 5c) the edge state density for $\Delta_{SAS} = 4.5$ meV that corresponds to $M = -$0.45 meV, around 4-times larger $M$ than for $\Delta_{SAS} = 5.2$ meV. The density here shows an oscillation period close to twice as large, reflecting that oscillations are dominated by the quantity $\sqrt{M/B}$, see Eq. (11).

A potential drawback of our proposal is the relative small size of the gap $2A\sqrt{M/B} \approx 0.1$ meV. However, what mitigates this is the improved transport properties of high quality In$_x$Ga$_{1-x}$As materials, as compared to HgTe based systems. Enhancement of the gap can be achieved by lowering $\Delta_{SAS}$ thereby easily doubling $M$; the band inversion anticrossing can then be pushed to higher values of $k$ thus increasing the size of the anticrossing gap. By optimizing the superlattice parameters and the bilayer setup one could anticipate an increase in $A$ by a factor of 2. An additional enhancement is obtained by decreasing the superlattice period down to e.g. $L = 40$ nm. Hence by optimizing the system parameters the gap could be pushed to $\sim 1.5$ meV, thus lowering the requirements on the sample mobility and temperature of the experiments [22]. Further experiments based on detecting the edge transport [23] and scanning gate microscopy that can image the modulation of the edge charge density profile [24] are feasible.

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