Helical edge and surface states in HgTe quantum wells and bulk insulators

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The quantum spin Hall (QSH) effect is the property of a new state of matter which preserves time-reversal, has an energy gap in the bulk, but has topologically robust gapless states at the edge. Recently, it has been shown that HgTe quantum wells realize this novel effect. In this work, we start from realistic tight-binding models and demonstrate the existence of the helical edge states in HgTe quantum wells and calculate their physical properties. We also show that 3d HgTe is a topological insulator under uniaxial strain, and show that the surface states are described by single-component massless relativistic Dirac fermions in 2 + 1 dimensions. Experimental predictions are made based on the quantitative results obtained from realistic calculations.

PACS numbers: 72.15Gd, 73.63.Hs, 75.47.-m, 72.25.-b

Conventional insulators have a gap for all charge excitations and their physical properties are not sensitive to changes in the boundary conditions. Recently, a new class of quantum spin Hall (QSH) insulators has been proposed theoretically in both 2d and 3d. The QSH insulators are invariant under time reversal, have a charge excitation gap in the bulk, and have topologically protected gapless edge states that lie in the bulk insulating gap. This type of insulator is typically realized in spin-orbit coupled systems; and the corresponding edge states have a distinct helical property: states with one spin-orbit coupling move around the sample edge in one direction, while states with the opposite spin-orbit coupling move in the opposite direction. The helical edge states are responsible for the intrinsic spin Hall effect in spin-orbit coupled systems; and the corresponding edge states have a similar distinction and is the natural generalization of the QSH insulator.

The study of the QSH effect in quasi-2d HgTe/CdTe quantum wells carried out in Ref. is based on a simplified model obtained by perturbation theory and the envelope function approximation. The conclusion of a topological quantum phase transition is reached based on a Dirac-type subband level crossing at the Γ point. However, such a level crossing is not generic and could be avoided in the real system due to the bulk inversion asymmetry (BIA) of the zinc-blende lattice. Consequently, a more realistic study is necessary to obtain a better understanding of the QSH phase and the topological phase transition. In this paper, we study the subband structure and edge state properties of HgTe/CdTe quantum wells using a realistic tight-binding (TB) model. The level crossing avoided at the Γ point is recovered at several finite wavevectors. In other words, the phase transition between different insulating regions remains robust despite inversion symmetry breaking. Furthermore, the topological nature of the QSH regime is demonstrated explicitly by studying the properties of the helical edge states in an open boundary system. We also apply the same realistic TB calculations to uniaxial strained 3d HgTe, and obtain the topologically non-trivial surface states. Thus, strained bulk HgTe is demonstrated to be a strong topological insulator. Ref. investigates a class of models with bulk inversion symmetry which strictly speaking does not apply to HgTe, however, adiabatic continuity is used to argue that strained bulk HgTe could be a strong topological insulator.

The CdTe and HgTe materials have the same zinc-blende lattice structure and are well-described by the same type of tight binding Hamiltonian, albeit with different parameters. This Hamiltonian includes two s-type orbitals and three p-type orbitals on each atom and reads

\[
H = \sum_{i\sigma R} E_{iR} c_{i\sigma R}^\dagger c_{i\sigma R} + \sum_{i\sigma R} E_{i\ell R} c_{i\sigma R}^\dagger c_{i\sigma \ell R} + \sum_{\vec{R}, \vec{R}'} V_{i\ell R}^c a_{i\sigma \vec{R}}^\dagger c_{i\sigma \vec{R}'} + H.C.
\]

(1)
where $a^\dagger_{\sigma R}$ and $c^\dagger_{\sigma R+\delta}$ are the creation operators for electrons on the anion and cation sites respectively, $i = (s, s', p_x, p_y, p_z)$ is the orbital index, and $\sigma$ is the spin index. $E_{i,a}, E_{i,s}$ and $V_{i,j}$ are the tight binding parameters defined by Slater and Koster. Spin-orbit coupling is contained in the last two terms, and is represented by two coupling constants $\lambda_a$ and $\lambda_b$. The tight binding parameters are taken from Ref. [14] where they were determined by fitting to a first-principles calculation.

To obtain the boundary (edge or surface) states for quasi-2d HgTe/CdTe quantum well structures and for the bulk 3d materials, we apply the Green’s function method [15, 16] based on the TB model described above. For the quantum well system, we consider a symmetric HgTe/CdTe hetero-structure with a fixed interface predicted by the TB model [15, 16]. Spin-orbit coupling is contained in the last two terms, and is represented by two coupling constants $\lambda_a$ and $\lambda_b$. The tight binding parameters are taken from Ref. [14] where they were determined by fitting to a first-principles calculation.

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sity of states for a quantum well structure with 20 and 10 “half”-layers are plotted in Figs. 2(a) and (b) respectively. Sharp peaks appear in the gap for the quantum well with 20 half-layers and are absent in the 10 half-layer system. As required by time reversal symmetry (TRS), the energy levels at the Γ point must be doubly degenerate, but can be split at finite \( k_y \). The energy level splitting near \( k_y = 0 \) as a function of \( k_y \) is plotted in the inset of Fig. 2(a), which shows a perfect linear dispersion indicating a level crossing of the edge states at \( k_y = 0 \). The spin densities of states for two \( k_y \)'s with opposite signs are plotted in Fig. 2(c). If the chemical potential lies between the two peaks, only the lower branch of the edge states is occupied and a spin current will be carried by the edge states. With the recursion method we can also obtain the charge density of states on the inner layers away from the edge. In the inset of Fig. 2(c), we plot the height of the in-gap peak for \( k_y = 0 \) on the different layers, which decays very fast from the edge and thus demonstrates that the in-gap peak is produced by the edge states. Finally, we plot the edge state dispersion in Fig. 2(d) with a color intensity plot generated from the density of states. W e find that the edge states correspond to a dangling bond at each surface atom, and are thus strongly dependent on the details of surface physics, such as surface reconstruction and disorder. Since in the present paper we are only concerned about the topological properties, which are insensitive to the details of surface physics, we can choose a surface regularization that removes the trivial surface states and leaves only the topological ones. Therefore, we will focus on the interface between bulk HgTe and CdTe, where the dangling bonds of HgTe are coupled to CdTe so the trivial surface states vanish. Since CdTe can be adiabatically connected with vacuum by taking its band gap to infinity, the topological properties of HgTe/CdTe interface are determined by HgTe.

Since bulk HgTe is a semi-metal, we need to apply a

FIG. 1: (a) The subband splitting as the function of layer thickness at one of the crossing points \( k = (0.017, 0.008) \) \( \pi/a \). (Inset) Schematic diagram of all 8 crossing points in the 2d BZ. (b) The subband splitting as the function of layer thickness at the Γ point.

FIG. 2: (a) The density of states at the edge of the quantum well with layer thickness \( d = 20(a/2) \). (The inset plot shows the linear energy splitting of the edge states in the very small region near \( k_y = 0 \).) (b) The density of states at the edge of the quantum well with layer thickness \( d = 10(a/2) \). (c) The spin density of states at the edge of the quantum well with thickness \( d = 20(a/2) \). (The inset plot shows the decay of density of states at the peak energy of the spectra with \( k_y = 0 \).) (d) The intensity color plot on the energy-momentum plane for the density of states at the edge of the quantum well with thickness \( d = 20(a/2) \).
small compressive strain, along say the [001] direction, to make it an insulator\cite{11}. The tight binding parameters for the strained HgTe are obtained by fitting the LDA results from the plane wave pseudo potential method\cite{17}. In the present paper, we apply the constrain along the [001] direction (z-direction) and locate the $HgTe/CdTe$ interface along both the [100] (x-direction) and [001] directions. And for both cases, we find non-trivial surface states. In Fig. 3 we plot the charge density of states in a color intensity plot. The single pair of surface states is clearly seen in the bulk insulating gap and they cross at the $\Gamma$-point. There are no other surface states in the entire zone. Any pure 2d band theory that respects TRS must have the same number of Kramers’s pairs on each of the time-reversal symmetric wave vectors because all of the $2N$ energy bands must be paired on these wavevectors. As a result, the 2d surface states of HgTe cannot emerge from any pure 2d surface effect, and only as a consequence of bulk topology.

It is useful to try to understand this result from a continuum $k \cdot P$ perspective. HgTe has a non-trivial topology because the band-structure is only “inverted” near the $\Gamma$-point. The fact that an occupied band at this point has $\Gamma^6$ character means that the $Z_2$ invariant picks up an extra factor of $(-1)$ (if we ignore the small BIA) making it non-trivial. Due to strong orbital mixing the $\Gamma^6$ character is washed out as one moves away from the $\Gamma$-point and at the special TR invariant points the “inverted” structure is absent. Therefore, we should be able to understand the topological properties from the band structure only near the $\Gamma$-point. The key point is to consider the full 6-band Kane model\cite{19} instead of just the reduced 4-band Luttinger model\cite{20}. If we only keep the bands in the Luttinger model the topological structure is absent. In the presence of uniaxial compressive strain along the (001) direction an insulating gap opens between the heavy-hole(HH) and light-hole(LH) bands by pushing the HH band downward in energy. For a movement we will ignore the HH band and focus only on the LH and $\Gamma^6$ (E) band. From the form of the Kane model, the coupling of the LH and E bands near the $\Gamma$-point is exactly a 3d anisotropic massive Dirac Hamiltonian if we ignore BIA and keep the leading order in $k$. The Dirac Hamiltonian preserves parity symmetry and we can label the bands by parity eigenvalues. Since the coupling is linear there must be one even (doubly degenerate) and one odd (doubly-degenerate) band. We expect that when the odd parity band lies below the even band then there will be a non-trivial $Z_2$ invariant which indicates an odd number of pairs of surface states that cross at TR invariant points\cite{12}. The presence of the HH band will change the features of the spectrum but it does not change the presence of the surface states, or their protected crossing, as long as the strain induced gap is open. The system will remain a 3d topological insulator when the HH band is coupled, and when BIA terms are added, as long as the bulk gap does not close. To show evidence of our statements we solve the 6-band Kane model on a cylinder. First we solve the model with the HH band completely decoupled from the LH and E bands (Fig. 4a). Here the HH band remains flat and is split from the LH band by the strain induced gap. In the gap there are clear, linearly dispersing surface states which traverse the gap between the LH and E bands. Nothing occurs at the other special points in the BZ, therefore this is a strong topological insulator. Turning on the coupling to the HH band changes features of the band structure but does not change the topology of the state since the gap between the LH and HH bands never closes. It is clear from Fig. 4b that even when the HH band is fully coupled the system is still a strong topological insulator with surface states crossing at $\Gamma$.

This work is supported by the NSF under grant numbers DMR-0342832 and the US Department of Energy, Office of Basic Energy Sciences under contract DE-AC03-76SF00515, the MARCO Center on Functional Engineered Nano Architectonics (FENA), and the Knowledge Innovation Project of the Chinese Academy of Sciences.
[1] B. A. Bernevig, T. L. Hughes, and S.C. Zhang, Science 314, 1757 (2006).
[2] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005).
[3] B.A. Bernevig and S.C. Zhang, Phys. Rev. Lett. 96, 106802 (2006).
[4] L. Fu, C. Kane, and E. Mele, arxiv: cond-mat/0607699.
[5] J. E. Moore and L. Balents, arxiv: cond-mat/0607314.
[6] C. Wu, B.A. Bernevig, and S.C. Zhang, Phys. Rev. Lett. 96, 106401 (2006).
[7] C. Xu and J. Moore, Phys. Rev. B 73, 045322 (2006).
[8] S. Murakami, N. Nagaosa, and S.C. Zhang, Science 301, 1348 (2003).
[9] J. Sinova et. al., Phys. Rev. Lett. 92, 126603 (2004).
[10] S. Murakami, N. Nagaosa, and S.C. Zhang, Phys. Rev. B 69, 235206 (2004).
[11] S. Murakami, N. Nagaosa, and S.C. Zhang, Phys. Rev. Lett. 93, 156804 (2004).
[12] L. Fu and C. Kane, arxiv: cond-mat/0611341.
[13] J. Slater and G. Koster, Phys. Rev. B 94, 1498 (1954).
[14] A. Kobayashi, O. Sankey and J. Dow, Phys. Rev. B 25, 6367 (1982).
[15] J. K. M. S. I. Turek, V. Drchal and P. Weinberger, Electronic structure of disordered alloys, surfaces and interfaces, Kluwer Academic publishers, 1997.
[16] Garnett W. Bryant, Phys. Rev. B 35, 5547 (1987).
[17] Z. Fang and K. Terakura, J. Phys.: Cond. Mat. 14, 3001 (2002).
[18] R. Winkler, Spin-orbit coupling effects in two-dimensional electron and hole systems, Springer Tracts in Modern Physics, 2003.
[19] E.O. Kane, J. Phys. Chem. Solids 1, 249 (1957).
[20] Y.R. Lin-Liu and L.J. Sham, Phys. Rev. B 32, 5561 (1985).