Topological phase transition HgTe Quantum Wells

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Abstract

Mercury telluride-cadmium telluride semiconductor quantum walls can change to Z_2 topological insulator phase from conventional insulator phase when the thickness of the quantum well is varied to the critical thickness d_c. In this report, I will introduce that Z_2 topological insulator is protected by time reversal symmetry and discuss to topological quantum phase transition between conventional insulators and topological insulators.

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I. INTRODUCTION

In 2005 Kane and Mele [7] first proposed a new kind of two dimensional insulating state without a magnetic field. And topological insulators were discovered. The main idea of topological insulators is that we started very simple Hamiltonian without complicated interactions. In the system, we get the hallmark topological number which is invariant under some perturbation. From the simple system we can get the same properties to a complicated one because it is topologically protected. Although those topological number is hard to change, it varies by some tremendous physical adjustment, such as a magnetic field. This phenomena can be thought as one of Quantum Phase Transition. In this paper, we discuss the CdTe/HgTe/CdTe quantum well transit from trivial insulator to Z_2 topological insulator by adjusting the thickness of HgTe sample in the middle.

The remaining parts of the paper are organized as follows. In Sec.II, we introduce Quantum Phase Transition and distinguish it from phase transition. In Sec.III, we discuss the physical meaning Chern number and find its relation with edge states. In Sec.IV, we calculated a graphene strip with spin orbit coupling under Time Reversal Symmetry. It brings Quantum Spin Hall Effect, Z_2 topological insulator. In Sec.V, we discuss Quantum Phase Transition of the CdTe/HgTe/CdTe quantum well between conventional insulator and topological insulator.

II. QUANTUM PHASE TRANSITION

Quantum phase transition is a phase transition at zero temperature due to Quantum fluctuation[11]. It is different with a classical phase transition, which occurs at nonzero temperature due to thermal fluctuation. Quantum phase transitions can only occur through changing a physical parameter, such as magnetic field. Quantum Hall effect and Quantum Spin effect are great example that we will discuss later.

Consider a Hamiltonian $H(g)$ for any lattice model to interpret Quantum Phase Transition. And g is a function of a dimensionless coupling. $H(g) = H_0 + gH_1$, where we assume H_0 and H_1 commute. This means that the eigenstates of H_0 are independent of g even though the eigenvalues vary with g. If we turn on g from 0, like turn on magnetic field, the ground state of H_0 evolves. There can be a level-crossing where an excited level becomes the ground state and the original ground state becomes a excited state at $g = g_c$. This implies that if Quantum Phase transition occurs, there is a level-crossing between one filling state and one unoccupied state. In many body wavefunction language, at zero temperature the fermi energy separating occupied states and unoccupied states. There is a level-crossing between those two kinds of the states, which means the energy spectrum is 'gapless'. Then gapless states appear if and only if Quantum Phase Transition occurs. We will use this idea to discuss Quantum Hall Effect.

III. INTEGER QUANTUM HALL EFFECT

A. Hall conductivity and Chern number

Thouless *et al* [13] discovered the topological structure of Hall conductance: they used the Kubo formula to get Hall conductivity σ_{xy} in the unit e^2/h is an expression of a topological invariant, Chern number. This physical quantity is insensitive to the details of material's band structure, for the mathematical reason that although the fiber bundle changes the shape, the twisted status is unchanged. Physically, Chern number is defined by Bloch wavefunction as.

$$C = \frac{1}{2\pi i} \int_T dk_x dk_y [< \partial_{k_x} u | \partial_{k_y} u > - < \partial_{k_y} u | \partial_{k_x} u >] \tag{1}$$

where u is single particle Bloch wavefunction. We often think that T is the first Brillouin zone. This equation also can be written by many-body Bloch wavefunction.

B. Number of edge state modes and Chern number

For Quantum Hall Effect, we add magnetic field in the sample so that free electrons rotate like cyclotrons. For this reason, charge current will accumulate around the edges of the sample so there is charge current cycling around the edges. These cycling electron states are called edge states. In general, the number of edge state modes, connecting conduction bands to valence bands, equals Chern number [2]. Here we pick up a specific example[5] to check this statement. Now we consider 2-D sample with square lattice and the Hamiltonian is defined as

$$\mathcal{H}(x,y)=\sum_n[C_n^\dagger\frac{\sigma_z-i\sigma_x}{2}C_{n+\hat{x}}+C_n^\dagger\frac{\sigma_z-i\sigma_y}{2}C_{n+\hat{y}}+h.c.]+m\sum_n C_n^\dagger\sigma_z C_n \tag{2}$$

Where n is lattice index and $\hat{x}$ and $\hat{y}$ means lattice shifts one side in x and y directions respectively. Also $C_n=(c_{n\uparrow}\ c_{n\downarrow})^T$. m is external magnetic field in z direction. We Fourier transform the Hamiltonian from position space to momentum space.

$$H(\vec{p})=\sum_{\vec{p}}c_{\vec{p}}^\dagger[\sin p_x\sigma_x+\sin p_y\sigma_y+(2-m-\cos p_x-\cos p_y)\sigma_z]c_{\vec{p}} \tag{3}$$

Use Kubo formula to calculate Hall conductivity and set $e^2/h=1$

$$\sigma_{xy}=\left\{\begin{matrix}-1 & 0<m<2\\ 1 & 2<m<4\\ 0 & \text{otherwise}\end{matrix}\right\} \tag{4}$$

Therefore, the value of m can control the value of the Hall conductivity. This means that external magnetic field changes quantum phase. To find edge states at $x=0$, we require $m=-1$ for $x<0$ and $m=1$ for $x>0$. Because there are two different quantum phases, $\sigma_{xy}=0\ and\ -1$, we are checking whether the edge states are gapless, to consist with Quantum Phase Transition occurring at $x=0$. For this definition, p_x is not good quantum number anymore but we can keep p_y. We also approximate $\mathcal{H}$ near $x=0$. The Hamiltonian is expressed as

$$\mathcal{H}(p_y)=-i\frac{\partial}{\partial_x}\sigma_x+p_y\sigma_y+m(x)\sigma_z \tag{5}$$

First, assume $p_y=0$ at $x=0$ (interface). The wavefunction $\psi=\exp(-\int_0^x m(x')dx')\phi_0$. Here we can put a minus or plus sign in front of the integral then get mathematically correct wavefunction. However, putting a plus sign is unphysical because wavefunction goes to infinity as $x\to\pm\infty$.

$$E\psi=\mathcal{H}\psi=\begin{pmatrix}m & im\\ im & -m\end{pmatrix}e^{-\int_0^x m(x')dx'}\phi \tag{6}$$

The eigenenergy is zero, the eigenstate $\phi=(1\ i)^T$ Fortunately, ϕ is also an eigenstate of σ_y. Therefore, the Hamiltonian operating this wavefunction is

$$\mathcal{H}(p_y)\psi=p_y\psi \tag{7}$$

This is one gapless edge state mode connecting from conduction bands to valence bands. For this model, at $x = 0$ the difference of Hall conductivity is one matching one edge state mode. One Quantum Phase switches to other different quantum phase through a gapless state. In general, an number of the edge state modes is the value of Chern number.

IV. QUANTUM SPIN HALL EFFECT AND TOPOLOGICAL INSULATORS

A. Graphene with Spin Orbit Interaction

We start at Haldane [4] Graphene Model, which is anomalous Quantum Hall Effect. Graphene exhibits a nonzero quantization of the Hall conductance σ^{xy} in the absence of an external magnetic field. Later, Kane and Mele [6] introduce a second nearest neighbor spin orbit model in the Hamiltonian then they got Quantum Spin Hall Effect (QSHE).

$$\mathcal{H} = \sum_{<ij>\alpha} t c_{i\alpha} c^{\dagger}_{j\alpha} + \sum_{<<ij>>\alpha\beta} i t_2 \nu_{ij} s^z_{\alpha\beta} c^{\dagger}_{i\alpha} c_{j\beta} \tag{8}$$

t is coefficient of the nearest neighbor hopping. t_2 is coefficient of the second nearest neighbor hopping. i, j are site indices and α, β are spin indices. Here $\nu_{ij} = (2/\sqrt{3})(\hat{d}_1 \times \hat{d}_2) = \pm 1$, where $\hat{d}_1$ and $\hat{d}_2$ are unit vectors along the two bonds the electron traverses going from site i to j. If we only consider the nearest neighbor hopping ($t_2 = 0$), Dirac cone spectrum shows up near K and K' points FIG.(1)(a).

This Hamiltonian is Time Reversal Invariant(TRI) which implies the Hall conductance (Chern number) here is zero (Append.A). For Haldane Graphene model the Hamiltonian breaks time reversal symmetry by alternating magnetic field, so this Hall conductance is not zero. The first term is obviously unchanged under Time Reversal Operator ($\Theta = \sigma_y K,\ \sigma_y$ for spin index) [12] and the second is also unchanged after the calculation. One of the most important properties of this Θ is $\Theta^2 = -1$ because in this situation an electron with spin 1/2 rotates 360 degree then the wave function change the sign. Therefore, for bosons $\Theta^2 = +1$. This -1 implies that there are at least two different degenerate states in TRI Hamiltonian. TRI Hamiltonian means Θ and $\mathcal{H}$ commute, if $|\phi>$ is an eigenstate, $\Theta|\phi>$ is also an eigenstate. Because $\Theta^2 = -1$, we can prove that $|\phi>$ and $\Theta|\phi>$ are different states. First, assuming they are the same so $\Theta|\phi> = e^{i\delta}|\phi>$.

$$-|\phi> = \Theta^2|\phi> = \Theta e^{i\delta}|\phi> = e^{-i\delta}\Theta|\phi> \tag{9}$$

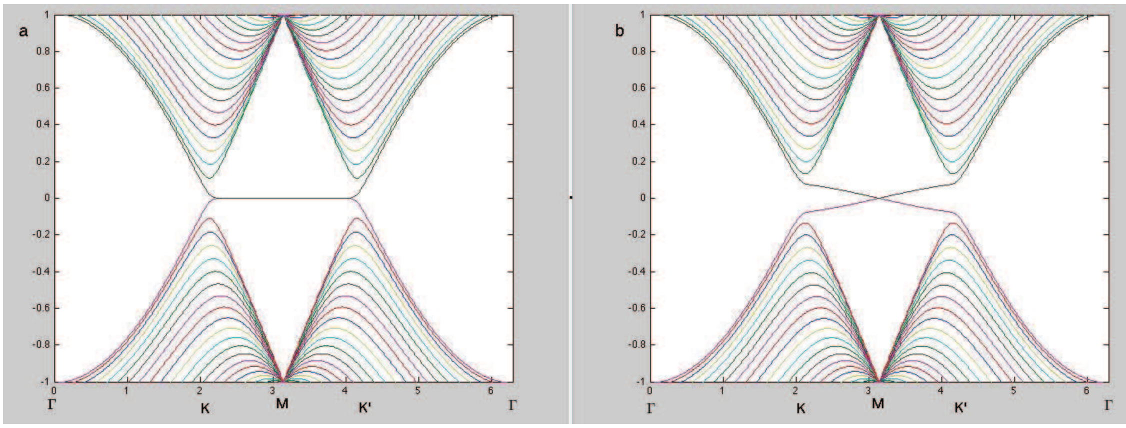

FIG. 1. Graphene Spectrum: the horizontal axis is momentum (k) in X direction (lattice constant = 1) and the vertical axis is Energy (E/t). (a) Spin orbit interaction is off. At $E = 0$, the flat spectrum from K to K' is actually four degeneracy states (two edges, two spin directions) which is the same with the analytic result of [10]. (b) Spin orbit interaction is on. $t_2 = 0.06t$ Near $E = 0$ and M point, each line represents two degenerate states in the two different edges.

It is a contradiction so they are different.

Now we solve this Hamiltonian for a graphene strip where the edges are along the zigzag direction. X direction of the strip is infinite, position space of x direction can be transform to momentum space. The two different edges are at $y = 0$ and $y = 80$ respectively. I recalculated[1] Kane's model and got more details of the energy spectrum.

In fig.1(a) (b), there are two degenerate gapless states at each edge between graphene and vacuum. These edge states give Quantum Phase Transition between graphene and vacuum.

In those spectrums, we can notice that there are two reflection symmetries. Up and down symmetry is consistent with Particle-Hole Symmetry. Left and right symmetry ($E(k) = E(-k)$) is consistent with Time Reversal Symmetry. In TRS, momenta at two mirror symmetry lines, Γ and M, are unchanged under Time Reversal Operation, this idea will be useful in 3-D topological insulator.

We calculate probabilities of the four states around $E = 0$ from M to K' and K points (Fig.2) and found that the four states near M are almost in the edges with extremely tiny probabilities in the bulk. At the point between M and K, the probabilities in the edges start to decrease and the particle has some chances to appear in the bulk. When momentum $k = 2\pi/3$ at K point, the states are totally in the bulk.

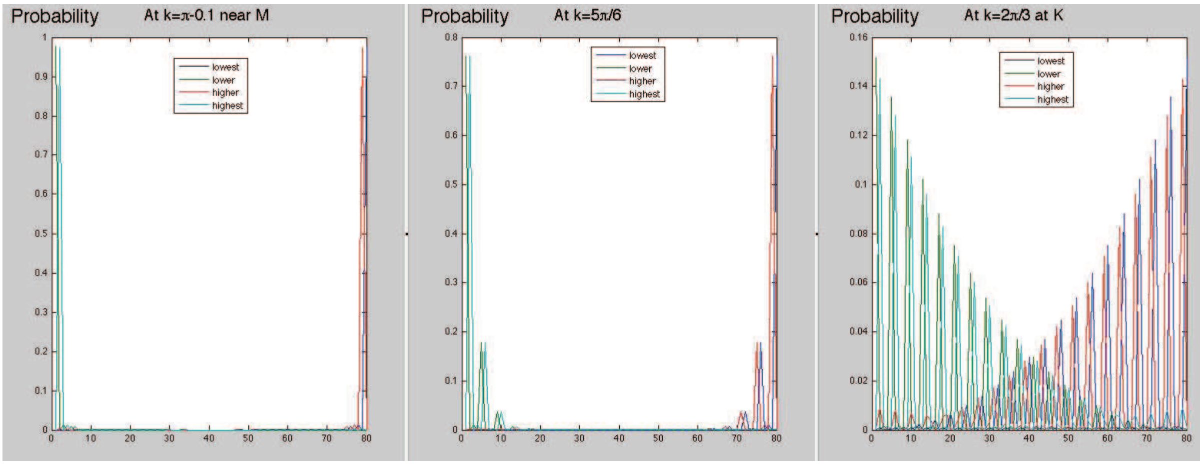

FIG. 2. The width of the sample is 80. The horizontal axis represents y position with spin index. Odd number of y is up spin and even number of y is down. The colors represent the different energy states.

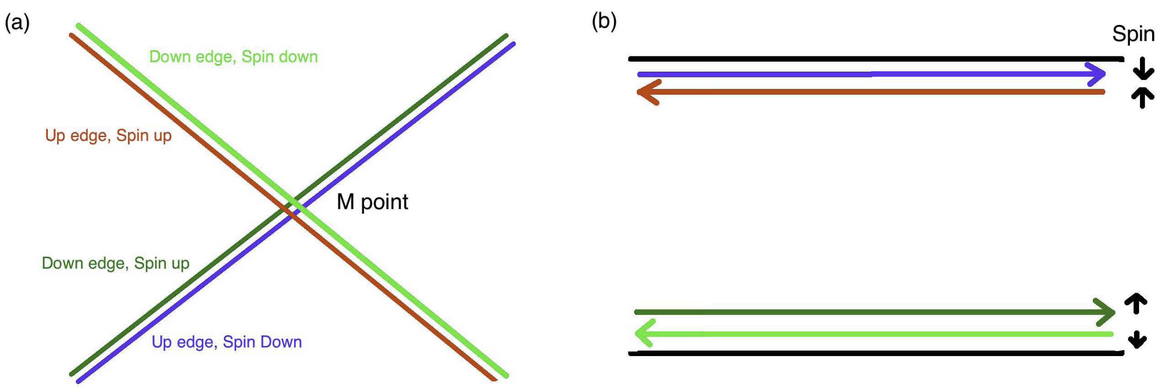

FIG. 3. (a) According to Fig.(2), we draw the status of the four states near M point. Actually, Two nearest line are overlapping. (b) There is spin current in the edges. One crossing represents one edge of spin current.

In Fig.(2), each state having pure up or down spin states is consistent with that $\hat{S}_z$ commutes with Hamiltonian. At lower temperature, Fermi energy is 0 so the states lower than M point are occupied. In the first Brilloun zone and Fig.(3)(a), the blue and dark green lines are half-filled with momenta $k > 0$ and the red and light green lines are half-filled also with momenta $k < 0$. Therefore, based on the momentum distribution, spin current propagates around the edges in a graphene strip(Fig.(3)(b)).

In general, there is the distinction between odd and even number of Kramer's pairs in the edges. There can be any number of crossings (Dirac cones) in the first Brillouin zone. Two

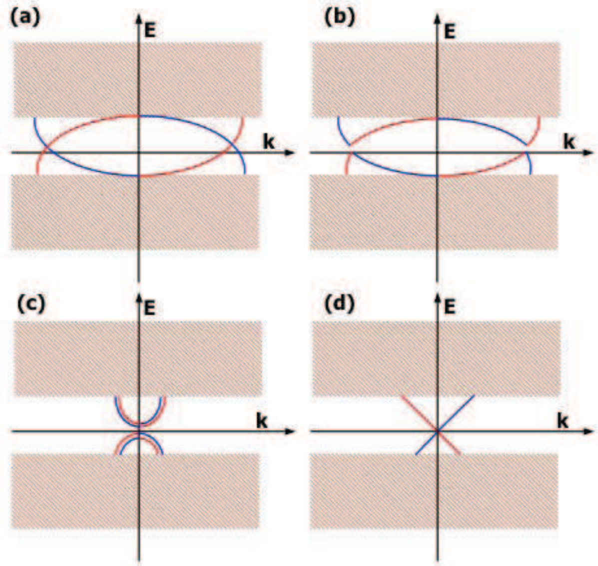

FIG. 4. [9] Brown areas are regions of bulk states. Red and blue dispersing edge states represent Kramers' partners (a)An even number of pairs of fermion branches crossing at k points which are the second kind of crosses. (b) A slight TRS perturbation added to the system causes the edge states are unstable to gap formation. (c) Two pairs of fermion branches that initially crossed at the special point $k = 0$ are shown after an infinitesimal perturbation is added. A gap is formed and TRS is kept but this configuration is also unstable to gap formation (d) A single pair of fermion branches crosses at $k = 0$. A perturbation cannot open a gap because in that case there would be two different states which were singly degenerate which will break TRS, thus this configuration is stable.

kinds of the crossings can be considered. First, one line of a crossing is a Kramer partner of the other line of the crossing with a mirror symmetry line at M and Γ point. For example, in this graphene strip, the red and blue (light and dark green) lines are a Kramer pair. Second, One cross is a Kramer partner of another crossing with the same symmetry line. TRS perturbation is added to the system. An even number of Kramer pairs open a gap easily which still keeps Time Reversal Invariance (Fig.(4)). For an odd number of kramer pairs, there must exist an odd number of the first kind of crossings. First, consider one crossing is in one edge. Because $\Theta^2 = -1$ for fermions, at a mirror symmetry lines K or Γ, two different states are Kramer partners. If a gap is opened, one state goes down and the other goes up for continuity. This breaks TRS because their partners' energy becomes different. To keep

TRS, this crossing should be locked under any TSI perturbation. Likewise, odd number of crosses is kept odd without breaking TRS.

This is called topological insulator and different from conventional insulator with all gap states. (Although superconductor has gaps, we don't consider this situation.) Here some of the edge states are not gapped depending on perturbation so topological insulator is not exactly like conventional conventional but is more like semimetal. Even and odd number of kramers' pairs are topologically protected by Time Reversal Symmetry. We called that topological insulator with odd pairs is nontrivial because it always has spin current around the edges (Quantum Spin Hall Effect) and it with even pairs is trivial because spin current disappears easily due to arbitrary TSI perturbation. Therefore, we define $\mathcal{Z}_2 = \{0, 1\}$ for even and odd pairs respectively. It is like Integer Quantum Hall Effect with Chern number $\mathcal{Z}$ or the TKNN integer [13] [8](Hall conductance). Originally any number of gapless states can give Quantum Phase Transition but for Time Reversal Symmetry, only odd number of pair fermion crossings can get Quantum Phase transition.

V. TOPOLOGICAL PHASE TRANSITION IN HGTE QUANTUM WELLS

Unfortunately, the striking proposal of the QSH in graphene [7] is hard to be observed due to the extremely small spin-orbit interaction ($\sim 10^{-3} meV$). However, Bernevig, Hughes, and Zhang proposed the HgTe/CdTe Quantum Wells as a candidate of the QSH [3]. We will follow this paper [3] to introduce the candidate of the QSHE.

We consider the band spectrum of CdTe and HgTe to discuss that the gapless states cause Quantum Phase Transition. The main point of the QSHE is to discuss the band crossing at the symmetry points $((k_x, k_y) = (0, 0) = (\pi, 0) = (0, \pi) = (\pi, \pi)$ because Karmers' pairs stay together at those points.) Here, we consider only the bands near the Γ point $(0, 0)$ and in this case the other points are irrelevant. Both Γ_8 and Γ_6 are in CdTe and HgTe. For CdTe the energy of Γ_8 band is lower than Γ_6 band. For HgTe, the energy order switches in Fig.5. Therefore, we can use two CdTe materials to sandwich HgTe and adjust the thickness d of the HgTe material. When $d = d_c$ at Γ point Γ_8 and Γ_6 touch, those two states becomes the gapless states. We know in Fig.5 that when $d > d_c$, the Γ_8 band lies below the Γ_6 band. In the two other sides of CdTe, the energy of the Γ_6 is higher. Therefore, at the edges HgTe, those two bands might touch as gapless states. (I will prove it later.) This result is similar

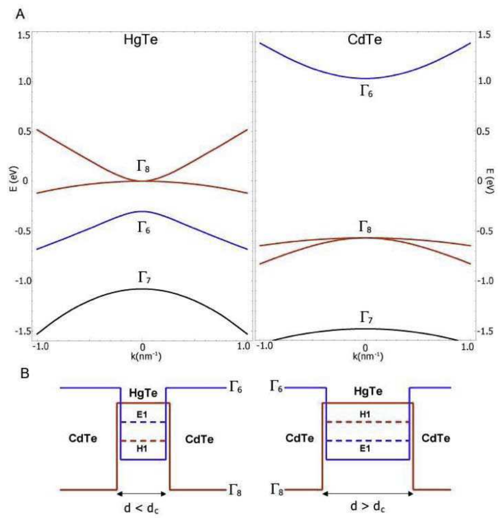

FIG. 5. [3] (A) HgTe and CdTe bulk energy bands near the Γ point (B) In the system of the CdTe/HgTe/CdTe quantum well as $d < d_c$, $E1(\Gamma_6) > H1(\Gamma_8)$ and as $d > d_c$, $E1(\Gamma_6) < H1(\Gamma_8)$.

with the previous section. There are some gapless states at the edges so this graphene is topologically nontrivial, QSHE. Here because the band crossings are at some certain place, 'unrigorously' HgTe/CdTe Quantum wells is topologically nontrivial, QSHE.

HgTe/CeTe should be discussed strictly under time reversal symmetry with Z_2 topological signature. For the four bands model [3], including the spins, the Hamiltonian can be written down in the basis of $|\Gamma_6, 1/2>, \ |\Gamma_8, 3/2, \ |\Gamma_6, -1/2>, \ |\Gamma_8, -3/2>$

$$H_{eff}(k_x, k_y) = \begin{pmatrix} H(k) & 0 \\ 0 & H^*(k) \end{pmatrix}, \ H = \epsilon(k) + d_i(k)\sigma_i \tag{10}$$

,where $d_1 + id_2 = A(k_x + ik_y), \ d_3 = M - B(k_x^2 + k_y^2), \ \epsilon_k = C - D(k_x^2 + k_y^2)$. We can verify this Hamiltonian satisfies Time Reversal Symmetry. i.e.

$$(\mathbb{I} \otimes \sigma_y)H^*(k)(\mathbb{I} \otimes \sigma_y)^{-1} = H(k) \tag{11}$$

Gap parameter M plays an important role here. M means the energy difference of Γ_6 and Γ_6 ,so when these two bands touch, M changes the sign. We can use the similar method in Sec.III B to compute the Hall conductance for 2×2 sub-block $H(k)$ in H_{eff}. Therefore, the Hall conductance changing $\Delta\sigma_{Hxy}$ between HgTe and the vacuum is 1. Because the whole system keeps Time Reversal Symmetry, the total Hall conductance vanishes (Append.A). This means the Hall conductance $\Delta\sigma_{H^*xy}$ for $H^*(k)$ is -1. But if we consider the spin Hall conductance $\Delta\sigma^s_{xy}$, $\Delta\sigma_{H^*xy}$ should change the sign because H^* is the basis with the negative spins. Therefore, the spin Hall conductance for HgTe is $\Delta\sigma^s_{xy} = \Delta\sigma_{H^xy} + \Delta\sigma_{H^*xy} = 2$. It implies that the edge states between the vacuum and HgTe include only one crossing gapless states (one left-chiral and one right-chiral are a kramers' pair). There is a quantum phase transition between HgTe and the vacuum. The vacuum is obviously topologically trivial so HgTe is topologically non-trivial in $\mathbb{Z}_2$. As $d > d_c$, the HgTe/CeTe Quantum well has Quantum Spin Hall Effect.

VI. CONCLUSION

The Quantum Phase Transition between topological insulator and conventional insulator can be determined by even or odd number of the gapless cross states between the two phases. If there is an odd number of the states in the boarder, conventional insulator in one side and topological insulator is in the other side. For an even number of the state, these two phases will be the same. Therefore, we used the number of the gapless states argument to discuss the topological non-trivial property of the CdTe/HgTe/CdTe quantum well. We found as $d > d_c$, this quantum is Z_2 topological insulator under time reversal symmetry. In addition, in experiment $d_c \sim 64\mathring{A}$.

Appendix A: Hall conductance vanishes under time reversal symmetry

We define Ω as

$$\Omega(\vec{k}) =< \partial_{k_x}|\partial_{k_y} > - < \partial_{k_y}|\partial_{k_x} > \tag{A1}$$

When integrate Ω in the first Brillouin zone, we get Chern number by Eq.1. If Hamiltonian has TRS and Parity (for normal samples always have parity), Ω is invariant. Therefore, under parity $\vec{k} \to -\vec{k}$, $\Omega(\vec{k}) = \Omega(-\vec{k})$. For TRS, we know Θ is an antiunitary operator so $<\Theta\alpha|\Theta\beta> (\hat{k}) =< \beta|\alpha> (-\hat{k})$. It implies that $\Omega(\hat{k}) = -\Omega(-\hat{k})$. Finally, $\Omega(-\hat{k}) = -\Omega(\hat{-k})$ so under TRS and Parity Ω is zero. Hall conductance vanishes.

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