



Supporting Online Material for

**Quantum Spin Hall Effect and Topological Phase Transition in HgTe
Quantum Wells**

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SOM Text

Table S1

Fig. S1

References

1 Envelope functions at $\mathbf{k}_{\parallel} = 0$

We show that our effective Hamiltonian can be derived perturbatively with $\mathbf{k} \cdot \mathbf{P}$ theory and is a quantitatively accurate description of the band structure for the $E1$ and the $H1$ subband states. We start from the 6-band bulk Kane model which incorporates the Γ_6 and Γ_8 bands but neglects the split-off Γ_7 band(the contribution of the split-off band to the $E1, H1$ energies is less than 5%(S2)):

$$\mathcal{H}(\vec{k}) = \begin{pmatrix} E_c I_{2 \times 2} + H_c & T_{2 \times 4} \\ T_{4 \times 2}^\dagger & E_v I_{4 \times 4} + H_v \end{pmatrix} \quad (1)$$

where E_c is the conduction band offset energy, E_v is the valence band offset energy, H_c, H_v are the conduction and valence (Luttinger) band Hamiltonians, while $T(k)$ is the interaction matrix between the conduction and valence bands:

$$H_c = \begin{pmatrix} \frac{\hbar^2 k^2}{2m^*} & 0 \\ 0 & \frac{\hbar^2 k^2}{2m^*} \end{pmatrix}; \quad T^\dagger = \begin{pmatrix} -\frac{1}{\sqrt{2}} P k_- & 0 \\ \sqrt{\frac{2}{3}} P k_z & -\frac{1}{\sqrt{6}} P k_- \\ \frac{1}{\sqrt{6}} P k_- & \sqrt{\frac{2}{3}} P k_z \\ 0 & \frac{1}{\sqrt{2}} P k_- \end{pmatrix}$$

$$H_v = -\frac{\hbar^2}{2m_0}(\gamma_1 + \frac{5}{2}\gamma_2)k^2 + \frac{\hbar^2}{m_0}\gamma_2(\vec{k} \cdot \vec{S})^2 \quad (2)$$

where m^* is the effective electron mass in the conduction band, $k_{\pm} = k_x \pm i k_y$, $P = -\frac{\hbar}{m_0} \langle s | p_x | X \rangle$ is the Kane matrix element between the s and p bands with m_0 the bare electron mass, \vec{S} is the spin-3/2 operator whose representation are the 4×4 spin matrices, and γ_1, γ_2 are the effective Luttinger parameters in the valence band. The ordered basis for this form of the Kane model is $(|\Gamma_6, +1/2 \rangle, |\Gamma_6, -1/2 \rangle, |\Gamma_8, +3/2 \rangle, |\Gamma_8, +1/2 \rangle, |\Gamma_8, -1/2 \rangle, |\Gamma_8, -3/2 \rangle)$. Although due to space constraints the above Hamiltonian is written in the spherical approximation, our calculations include the anisotropy effects generated by a third Luttinger parameter $\gamma_3 \neq \gamma_2$. The quantum well growth direction is along z with $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ for $z < -d/2$, HgTe for $-d/2 < z < d/2$ and $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ for $z > d/2$. Our problem reduces to solving, in the presence of continuous boundary conditions, the Hamiltonian Eq. 1 in each of the 3 regions

of the quantum well. The material parameters E_c , E_v , $\gamma_{1,2,3}$, and m^* , are discontinuous at the boundaries of the 3 regions, taking the $\text{Hg}_{1-x}\text{Cd}_x\text{Te}/\text{HgTe}/\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ values (see Ref. (SI) for numerical values), so we have a set of 3 multi-component eigenvalue equations coupled by the boundary conditions. The in-plane momentum is a good quantum number and the solution in each region takes the general form:

$$\begin{aligned}\mathcal{H}(\vec{k})\psi(k_x, k_y, z) &= \mathcal{H}(k_x, k_y, -i\partial_z)\psi(k_x, k_y, z); \\ \psi(k_x, k_y, z) &= e^{i(k_x x + k_y y)}\Psi(z)\end{aligned}\quad (3)$$

where $\Psi(z)$ is the envelope function spinor in the six component basis introduced earlier.

We solve the Hamiltonian analytically by first solving for the eigenstates at zero in-plane momentum, and then perturbatively finding the form of the Hamiltonian for finite in-plane \mathbf{k} : $\mathcal{H}(k_x, k_y, -i\partial_z) = \mathcal{H}(0, 0, -i\partial_z) + \delta\mathcal{H}(k_x, k_y, -i\partial_z)$. At $k_x = k_y = 0$ we have the following Hamiltonian:

$$\mathcal{H}(0, 0, -i\partial_z) = \begin{pmatrix} T & 0 & 0 & \sqrt{\frac{2}{3}}P(-i\partial_z) & 0 & 0 \\ 0 & T & 0 & 0 & \sqrt{\frac{2}{3}}P(-i\partial_z) & 0 \\ 0 & 0 & U + V & 0 & 0 & 0 \\ \sqrt{\frac{2}{3}}P(-i\partial_z) & 0 & 0 & U - V & 0 & 0 \\ 0 & \sqrt{\frac{2}{3}}P(-i\partial_z) & 0 & 0 & U - V & 0 \\ 0 & 0 & 0 & 0 & 0 & U + V \end{pmatrix} \quad (4)$$

where $T = E_c(z) + (-\partial_z A(z)\partial_z)$, $U = E_v(z) - (-\partial_z \gamma_1(z)\partial_z)$, $V = 2(-\partial_z \gamma_2(z)\partial_z)$. These parameters are treated as step functions in the z -direction with an abrupt change from the barrier region to the well region.

A general state in the envelope function approximation can be written in the following form:

$$\Psi(k_x, k_y, z) = e^{i(k_x x + k_y y)} \begin{pmatrix} f_1(z) \\ f_2(z) \\ f_3(z) \\ f_4(z) \\ f_5(z) \\ f_6(z) \end{pmatrix}. \quad (5)$$

At $k_x = k_y = 0$ the f_3 and f_6 components decouple and form the spin up and down (\pm) states of the $H1$ subband. The f_1, f_2, f_4, f_5 components combine together to form the spin up and down (\pm) states of the $E1$ and $L1$ subbands. The linear-in- k_z operator $\sqrt{\frac{2}{3}}Pk_z$, in $\mathcal{H}(0, 0, -i\partial_z)$ forces the $|\Gamma_6, \pm\frac{1}{2}\rangle(z)$ and $|\Gamma_8, \pm\frac{1}{2}\rangle(z)$ components of the $E1$ band to have different reflection symmetry under $z \leftrightarrow -z$. The $|\Gamma_6\rangle$ band is symmetric in z (exponentially decaying in CdTe and a $\cosh(z)$ dependence in HgTe) while the $|\Gamma_8, m_J = \pm 1/2\rangle$ band is antisymmetric in z (exponentially decaying in CdTe and a $\sinh(z)$ dependence in HgTe). The opposite choice of symmetry under $z \rightarrow -z$ reflection leads to the $L1$ band. However, this band is far away in energy from both the $E1$ and the $H1$ bands, does not cross either of them in the region of interest(S2), and we hence discard it.

For the $E1$ band we take the ansatz, already knowing it must be an interface state(S2), to be:

$$\Psi_I = \begin{pmatrix} e^{\alpha z} C_1 \\ 0 \\ 0 \\ e^{\alpha z} C_4 \\ 0 \\ 0 \end{pmatrix}, \quad \Psi_{II} = \begin{pmatrix} (e^{\delta z} + e^{-\delta z}) V_1 \\ 0 \\ 0 \\ (e^{\delta z} - e^{-\delta z}) V_4 \\ 0 \\ 0 \end{pmatrix}, \quad \Psi_{III} = \begin{pmatrix} e^{-\alpha z} C_1 \\ 0 \\ 0 \\ -e^{-\alpha z} C_4 \\ 0 \\ 0 \end{pmatrix}. \quad (6)$$

If we act on this ansatz with the Hamiltonian we decouple the 6×6 matrix into two, coupled, one-dimensional Schrodinger equations:

$$T f_1(z) + \sqrt{\frac{2}{3}} P(z) (-i\partial_z) f_4(z) = E f_1(z) \quad (7)$$

$$\sqrt{\frac{2}{3}} P(z) (-i\partial_z) f_1(z) + (U - V) f_4(z) = E f_4(z) \quad (8)$$

where P, T, U, V are given above. Using the restrictions from the Hamiltonian, the continuity of each wavefunction component at the boundaries, and the continuity of the probability current across the boundary, we derive the following set of equations that determine α and δ as a function of E :

$$\frac{E_c^{(Cd)} - A^{(Cd)} \alpha^2(E) - E}{\sqrt{\frac{2}{3}} \frac{P}{i} \alpha(E)} = \frac{\sqrt{\frac{2}{3}} \frac{P}{i} \alpha(E)}{E_v^{(Cd)} + (\gamma_1^{(Cd)} + 2\gamma_2^{(Cd)}) \alpha^2(E) - E} \quad (9)$$

$$\frac{E_c^{(Hg)} - A^{(Hg)}\delta^2(E) - E}{\sqrt{\frac{2}{3}}\frac{P}{i}\delta(E)} = \frac{\sqrt{\frac{2}{3}}\frac{P}{i}\delta(E)}{E_v^{(Hg)} + (\gamma_1^{(Hg)} + 2\gamma_2^{(Hg)})\delta^2(E) - E} \quad (10)$$

where a parameter $X^{(Cd)}$ means the value of that parameter in the CdTe barrier material and $X^{(Hg)}$ is the value in the HgTe well material. Once we have $\alpha(E)$ and $\delta(E)$ we can use them to determine E through the following equation derived from the boundary conditions:

$$\frac{E_c^{(Cd)} - A^{(Cd)}\alpha^2(E) - E}{\alpha(E)} = -\tanh\left(\frac{\delta(E)d}{2}\right) \left(\frac{E_c^{(Hg)} - A^{(Hg)}\delta^2(E) - E}{\delta(E)}\right). \quad (11)$$

These rational transcendental equations are solved numerically to obtain the energy of the $E1$ subband at $k_x = k_y = 0$.

We can follow a similar procedure to derive the energy of the $H1$ subband. The heavy hole subband (at $k_x = k_y = 0$) completely decouples from the other bands and we have the one-dimensional, one-component Hamiltonian:

$$Hf_3(z) = E_v(z) - (\gamma_1(z) - 2\gamma_2(z))(-\partial_z^2)f_3(z) = Ef_3(z). \quad (12)$$

We have the wavefunction in three regions

$$\begin{pmatrix} \Psi_I(z) \\ \Psi_{II}(z) \\ \Psi_{III}(z) \end{pmatrix} = \begin{pmatrix} C_3 e^{\beta z} \\ V_3 \cos(\kappa z) \\ C_3 e^{-\beta z} \end{pmatrix} \quad (13)$$

where $\beta^2(E) = \frac{E - E_v^{(Cd)}}{\gamma_1^{(Cd)} - 2\gamma_2^{(Cd)}}$ and $\kappa^2(E) = \frac{E_v^{(Hg)} - E}{\gamma_1^{(Hg)} - 2\gamma_2^{(Hg)}}$. We can pick $C_3 = 1$ which gives us the relation

$$V_3 = \frac{e^{-\frac{1}{2}\beta d}}{\cos(\kappa(E)d/2)} \quad (14)$$

from the boundary condition at $z = -d/2$. Finally, we need to normalize the wavefunction to get the coefficients. The energy of this state is determined by considering the conservation of probability current across the boundary. The following equation is solved for the energy:

$$\frac{1}{(\gamma_1^{(Cd)} - 2\gamma_2^{(Cd)})\beta(E)} = \frac{1}{(\gamma_1^{(Hg)} - 2\gamma_2^{(Hg)})\kappa(E)} \cot(\kappa(E)d/2). \quad (15)$$

We repeat both of these processes on a state with only $f_2(z)$ and $f_5(z)$ non-zero and on a state with only $f_6(z)$ non-zero and to get the $E1^-$ and $H1^-$ bands respectively. We have the forms of these states at $k_x = k_y = 0$ and can use $k \cdot P$ perturbation theory to derive a two dimensional Hamiltonian near the Γ point in k -space.

2 Perturbation Theory and Effective Hamiltonian

Define an ordered set of basis vectors ($|E1, + \rangle, |H1, + \rangle, |E1, - \rangle, |H1, - \rangle$). We can write the effective Hamiltonian as:

$$H_{ij}(k_x, k_y) = \int_{-\infty}^{\infty} dz \langle \psi_j | H_{6 \times 6}(k_x, k_y, -i\partial_z) | \psi_i \rangle \quad (16)$$

where ψ_i is the i -th element of the basis set given above which will give a 4×4 effective Hamiltonian. The integrals must be split into the three regions defined above, and the parameters from each material must be accounted for in the Hamiltonian. This Hamiltonian depends on the quantum-well width d , and once d is specified we can numerically calculate the matrix-elements. It is important to note that $f_1(z), f_2(z), f_3(z), f_6(z)$ are symmetric with respect to z and $f_4(z), f_5(z)$ are antisymmetric in $z(S2)$ which is a useful simplification in performing the integrals. An example of one integral is of the form:

$$\begin{aligned} \int dz f_3^*(z) \{ \gamma_3(z), -i\partial_z \} f_4(z) = \\ \int dz \frac{1}{i} (2\gamma_3(z) f_3^*(z) \partial_z f_4(z) + f_3^*(z) f_4(z) \partial_z \gamma_3(z)). \end{aligned} \quad (17)$$

The functional form of $\gamma_3(z)$ is

$$\gamma_3(z) = \gamma_3^{(Cd)}(\theta(-d/2 - z) + \theta(z - d/2)) + \gamma_3^{(Hg)}(\theta(z + d/2) - \theta(z - d/2)). \quad (18)$$

The z -derivative acting on this function produces δ -function terms that contribute a term proportional to $(\gamma_3^{(Cd)} - \gamma_3^{(Hg)})$ to the integral which vanish when these material parameters are equal. The integral then has to be evaluated numerically.

$d (\text{\AA})$	$A(\text{eV})$	$B(\text{eV})$	$C(\text{eV})$	$D(\text{eV})$	$M(\text{eV})$
58	-3.62	-18.0	-0.0180	-0.594	0.00922
70	-3.42	-16.9	-0.0263	0.514	-0.00686

Table 1: Parameters for $\text{Hg}_{0.32}\text{Cd}_{0.68}\text{Te}/\text{HgTe}$ quantum wells.

After calculating the matrix-elements we are left with an effective Hamiltonian parameterized in the following way:

$$\mathcal{H}(k_x, k_y) = \begin{pmatrix} \epsilon_k + \mathcal{M}(k) & Ak_- & 0 & 0 \\ Ak_+ & \epsilon_k - \mathcal{M}(k) & 0 & 0 \\ 0 & 0 & \epsilon_k + \mathcal{M}(k) & -Ak_+ \\ 0 & 0 & -Ak_- & \epsilon_k - \mathcal{M}(k) \end{pmatrix} \quad (19)$$

where $\epsilon_k = C - D(k_x^2 + k_y^2)$, $\mathcal{M}(k) = M - B(k_x^2 + k_y^2)$, $k_{\pm} = k_x \pm ik_y$, and A, B, C, D, M depend on the specified quantum-well width. For values of these parameters at $d = 40\text{\AA}$ and $d = 70\text{\AA}$ see Table I. This Hamiltonian is block diagonal and can be written in the form

$$\mathcal{H}(k_x, k_y) = \begin{pmatrix} H(k) & 0 \\ 0 & H^*(-k) \end{pmatrix} \quad (20)$$

where $H(k) = \epsilon_k I_{2 \times 2} + d^a(k) \sigma^a$, with $d^1 = Ak_x$, $d^2 = Ak_y$, and $d^3 = \mathcal{M}(k) = M - B(k_x^2 + k_y^2)$.

Finally, we define a unitary transformation:

$$U = \begin{pmatrix} I_{2 \times 2} & 0 \\ 0 & -\sigma^z \end{pmatrix} \quad (21)$$

and take $U^\dagger H_{4 \times 4} U$ which reverses the sign of the linear k terms in the lower block and puts it \mathcal{H} into the form

$$\mathcal{H}(k_x, k_y) = \begin{pmatrix} H(k) & 0 \\ 0 & H^*(k) \end{pmatrix}. \quad (22)$$

U does not affect the z -direction of spin and simply rotates the x and y axes in the lower block of the Hamiltonian by π . The energy dispersions for these bands are given in Fig. 1 of the supporting online material for several values of d .

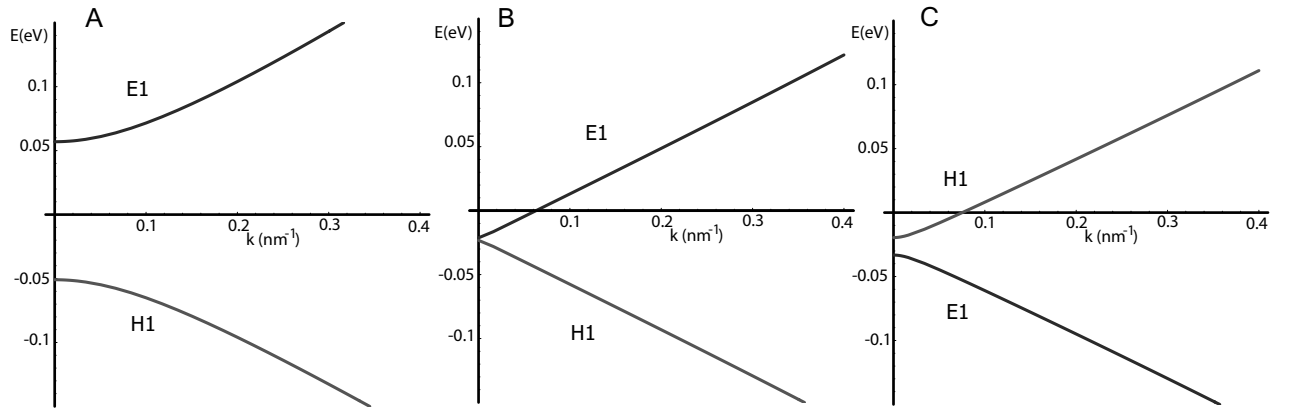


Figure 1: Dispersion relations for the $E1$ (blue) and $H1$ (red) subbands for (A) $d = 40\text{\AA}$ (B) $d = 63.5\text{\AA}$ (C) $d = 70\text{\AA}$.

Supporting References and Notes

S1. E.G. Novik *et. al.*, *Phys. Rev. B* **72**, 035321 (2005).

S2. A. Pfeuffer-Jeschke, Ph.D. Thesis, University of Wurzburg, Germany, 2000.