

Quantum Spin Hall Effect: a theoretical and experimental introduction at kindergarten level, non-shown version

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Historical consideration and Overview

Where everything get started

Theoretical: a picture

Preliminary

Graphene

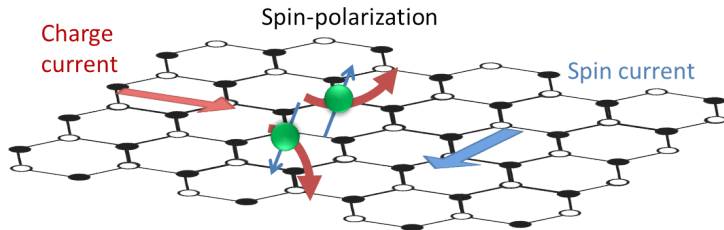
Famous Experiments

Quantum Spin Hall Insulator State in HgTe Quantum Wells

Supplementary Material

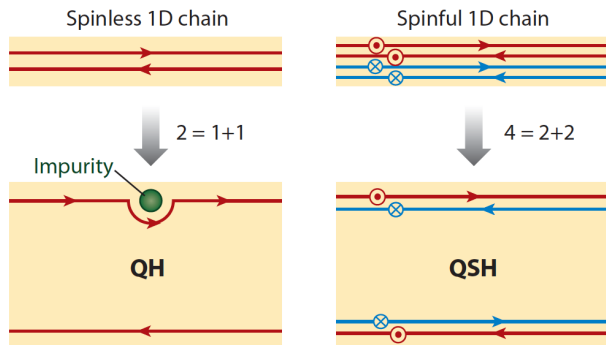
Spin Hall Effect?

M.I. Dyakonov and V.I. Perel in 1971 the phenomenon[1]. Cited by more than 732 times. J. E. Hirsch in 1999[2]. Cited by more than 1,031 times. Explained via s-o scattering. Qian Niu and A. H. MacDonald [3], intrinsic reason for this phenomenon. Cited by 1,123 times. Must in bulk-insulating material by Nagaosa, Murakami and ShouCheng Zhang [4] and cited by 207 times.



Why Spin Hall Effect

- ▶ Dissipationless quantum transport (unless TRS broken)[5]
(cited by 1,531 times.)



Berry Phase: a quick introduction

Here¹, we consider a adiabatic dynamical evolution under a parametric Hamiltonian $\mathcal{H}(\mathbf{R})$ on its n -th eigenstate, for a closed loop in parameter space:

$$|n(\mathbf{R}(t))\rangle = e^{i\theta} |n(\mathbf{R}(0))\rangle,$$

where the additional phase is partially due to dynamical term,

$$\theta = \frac{1}{\hbar} \int_0^t E_n(\mathbf{R}(t')) dt' - i \int_0^t \left\langle n(\mathbf{R}(t')) \left| \frac{d}{dt'} \right| n(\mathbf{R}(t')) \right\rangle$$

An additional topological term comes from the second term if the system is topological nontrivial. A straight forward way of such nontrivial Hamiltonian is $\mathcal{H}(\mathbf{R}) = \epsilon(\mathbf{R}) + \mathbf{R} \cdot \boldsymbol{\sigma}$ for a 2-state system.

¹For detailed information plz check my note of B.P via [this link](#)

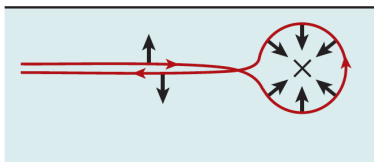
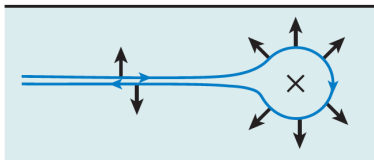
Chern Number is also derived based on this. First we can define a vector (Berry Curvature) \mathbf{V}_n for its i component is

$$V_{ni} = \text{Im} \sum_{m \neq n} \frac{\langle n(\mathbf{R}) | (\nabla_{\mathbf{R}} H(\mathbf{R})) | m(\mathbf{R}) \rangle \times \langle m(\mathbf{R}) | (\nabla_{\mathbf{R}} H(\mathbf{R})) | n(\mathbf{R}) \rangle}{(E_m(\mathbf{R}) - E_n(\mathbf{R}))^2}$$

and the nontrivial term, is

$$\gamma_n = - \iint_c d\mathbf{S} \cdot \mathbf{V}_n$$

Chern number is simply integration over a closed surface of such vector and divided by 2π . Note the relationship between Chern Number and Hall Conductance: $\sigma = \frac{e^2}{h} \cdot CN$. A good literature of this topic can be seen at [6].

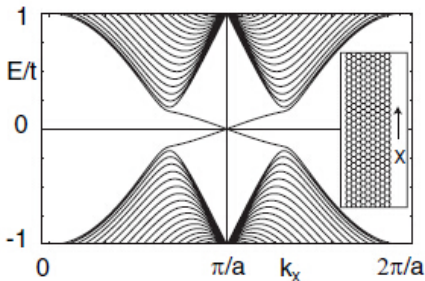


× Nonmagnetic impurity

Figure: TR protected impurity scattering with additional geometry phase 2π and interference cancel it (for spin, $\mathbf{V}_{\pm} = \pm \frac{\mathbf{R}}{2R^3}$, which gives a circle rotation of $\Omega = 2\pi$ yields $\gamma = \pi$, i.e., $e^{-i\gamma} = -1$)

Considering the work we have illustrated so far, the graphene is a good test platform. We have Kane-Mele Model for half-infinite case and yields edge state with chirality:

$E = -A s \sin(k_x)$ where s stands for spin². It's solvable and pointed out the requirement for the parameter.



²details see further section

Quantum spin Hall effect in graphene (Haldane, Kane&Mele)

- SO coupling opens up a gap at the Dirac point.
- One pair of TR edge state on each edge.
- Numerical calculation indicate stability (Sheng et al)

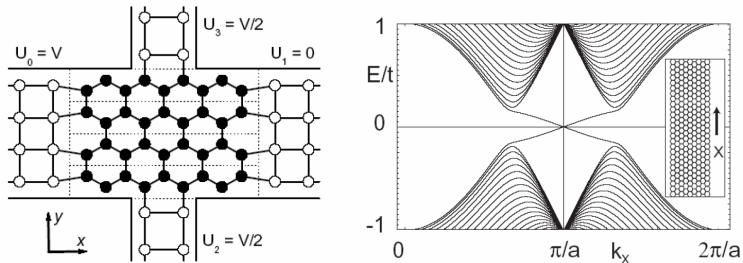


Figure: From S-C Zhang's Slides at 2005

A hint to solve (the Haldane model)

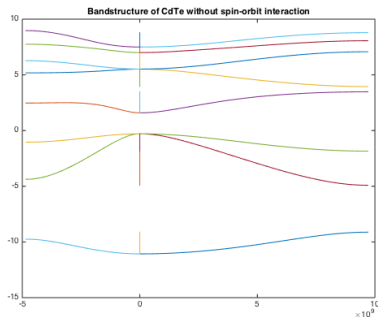
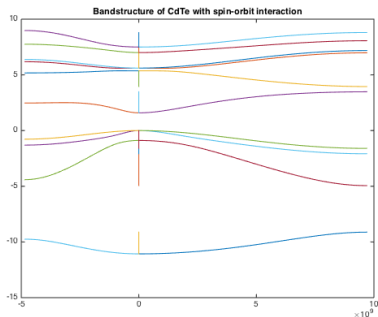
If you insist to know how to solve, there is a brief description and detailed information can be seen in my note as mentioned before.

1. Write down Hamiltonian, (for the sprite, we can suppose a simple cubic lattice). With fixed k_z , expand via Γ algebra and yield bulk energy $E = \pm \sqrt{\mathcal{M}^2(\mathbf{k}) + A^2(\sin^2 k_x + \sin^2 k_y)}$
2. Discrete for y direction is finite size and make fourier trans. $c_{k_x, k_y} = \frac{1}{L} \sum_j e^{ik_y j} c_{k_x, j}$ and write down Hamiltonian within this framework.
3. Use ansatz $\psi(k_x, j) = \lambda^{-j} \phi(k_x)$ and yield two eigenstate problem which is simply 4×4 case.

However graphene is disappointing, for its poor o-s coupling strength (Carbon is too light). All the hall phenomenon in graphene is summarized in YuanBo-Zhang's [7] (cited by 8,872 times.).

Now, we consider the famous experiment: S-C Zhang *et al*:
Quantum spin hall insulator state in HgTe quantum wells
[8](cited by 2,594 times).
Close to fermi level, there are 4 bands.

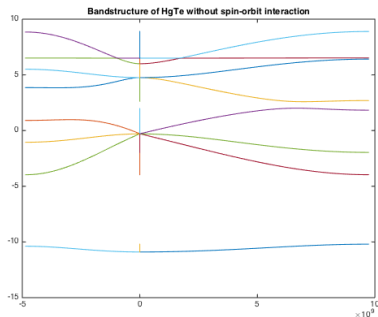
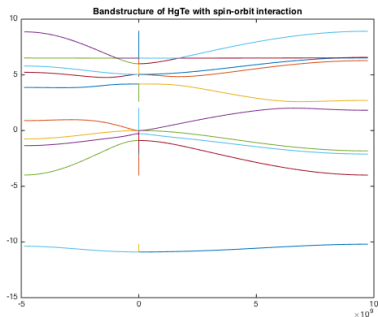
CdTe vs. HgTe, w/ or w/o s-o coupling³



s -like E_1 band lies above p -like H_1 band. Normal semiconductor.

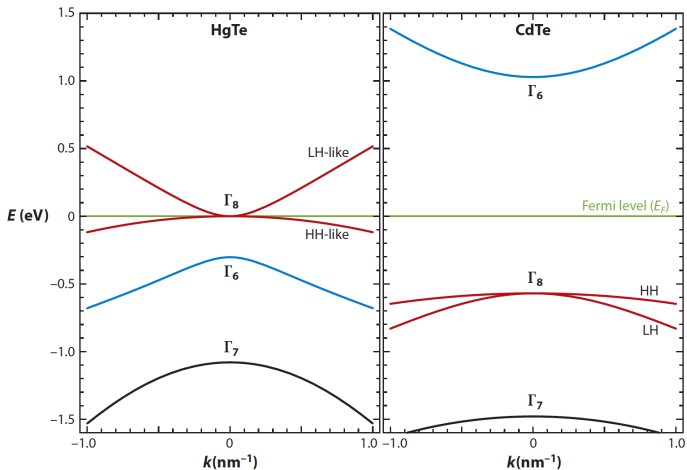
³Generated by MATLAB. Feel free to use my code. Using the Slater-Koster tight-binding method

CdTe vs. HgTe, w/ or w/o s-o coupling, cont.³



s -like E_1 band lies behind p -like H_1 band. Inverted semiconductor.

³Generated by MATLAB. Feel free to use my code. Using the Slater-Koster tight-binding method



A 'sandwich' QW might influence the 'inverty' of the HgTe band if thickness is not enough. We then can make a mathematical description based on taylor expansion near Dirac point of our system.

BHZ model (by symmetry arguments, Γ_6 odd, Γ_8 even). Basis are $|E^\pm\rangle^4$, $|H^\pm\rangle^5$. Just suit Haldane model well.

$$H_{\text{eff}}(k_x, k_y) = \begin{pmatrix} H(k) & 0 \\ 0 & H^*(-k) \end{pmatrix},$$

$$H(k) = \epsilon(k) + \mathbf{d}(k) \cdot \boldsymbol{\sigma}$$

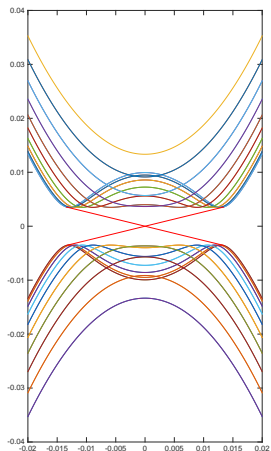


Figure: Calculation of Energy Band

⁴ $|E^+\rangle$: s-o state $|s, \uparrow\rangle$; $|E^-\rangle$: $|s, \downarrow\rangle$; $\Rightarrow |J = 1/2, m = \pm 1/2\rangle$

⁵ $|H^+\rangle$: s-o state $|p_x + ip_y, \uparrow\rangle$; $|H^-\rangle$: $| -p_x + ip_y, \downarrow\rangle$; $\Rightarrow |J = 3/2, m = \pm 3/2\rangle$

With analyzing and the material's property, we have really important information that

$d_3 = M - B(k_x^2 + k_y^2)$, M : the mass parameter in Dirac-description

CdTe: $M < 0$, HgTe: M might > 0 .

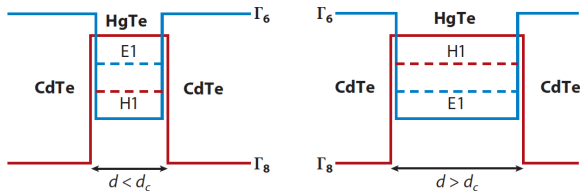
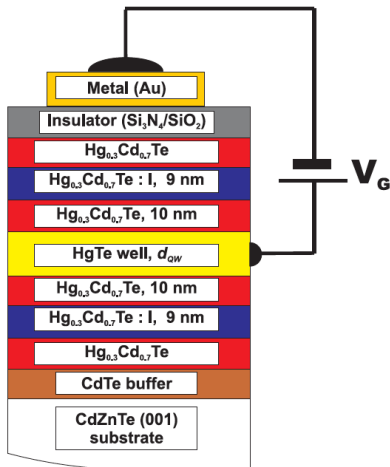
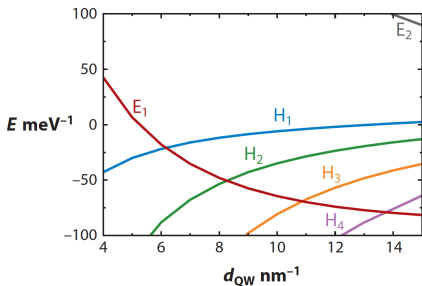


Figure: Energy Band for the connecting CdTe and HgTe. For $d_{QW} > d_c$ the HgTe layer becomes quantum spin Hall insulator. Massless helical states are confined on the sample edge. The sample has a finite conductance even when the Fermi level lies inside the bulk insulating gap.

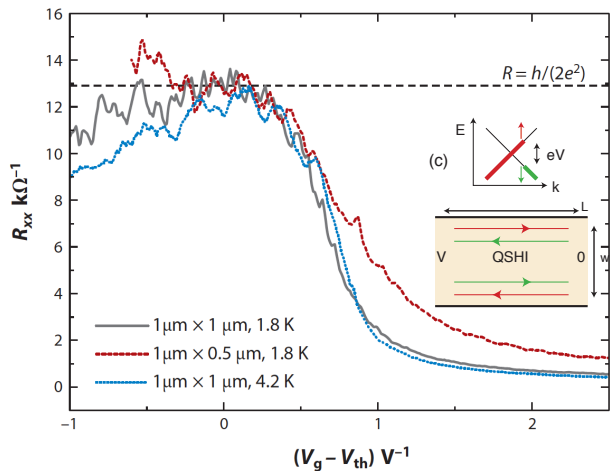
Hence if we make a Quantum Well with width d has a critical point d_c where if $d < d_c$, $M < 0$ and if $d > d_c$, $M > 0$ (for the influence of the 'sandwich cover'. Simulation with 8 bands $\mathbf{k} \cdot \mathbf{p}$ model of Hartree calculation [9] (cited by 2,665 times.) shows that $d_c = 6.3$ nm and confirmed by experiment.



A Landau level argument

$|J = 3/2, m = -3/2\rangle$ will earn negative energy from LL, while $|J = 1/2, m = 1/2\rangle$ will earn positive energy from LL. If $d > d_c$, for a particular $B = B_c$ the two subbands meet. This gives rise to a strong magnetic field recovery of Hall conductance $\sigma_{xy} = 0 \pm e^2/h$, + for conduction band and - for valence band. Higher field will then cancel it again and recover to $\sigma_{xy} = 0$. But this is hard to test from experiment.

Things to be measured: Longitude Resistance R_{xx}



Things to be measured: Four-term $R_{ij,kl}$

Landauer-Büttiker formalism, only valid for both-side⁶ edge-state transport.

$$I_i = \frac{e}{h} \sum_j (T_{ij}\mu_i - T_{ji}\mu_j)$$
$$T_{i,i+1} = T_{i+1,1} = 1$$
$$I_1 = -I_4 \equiv I_{14}$$
$$\mu_4 = 0 \quad \text{zero-point}$$
$$\begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \mu_5 \\ \mu_6 \end{pmatrix} = \frac{I_{14}h}{e} \begin{pmatrix} -3/2 \\ -1 \\ -1/2 \\ -1/2 \\ -1 \end{pmatrix}$$

⁶Simple Quantum Hall Effect doesn't have $T_{i+1,i} = 1$

$R_{ij,kl}$	Expected value
$R_{14,14}$	$3h/2e^2$
$R_{14,23}$	$h/2e^2$
$R_{13,13}$	$4h/3e^2$
$R_{13,56}$	$h/3e^2$

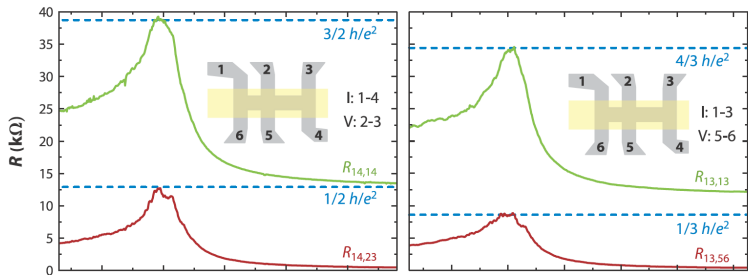


Figure: Four-term $R_{ij,kl}$ measurement with precise gating

Experiment Result

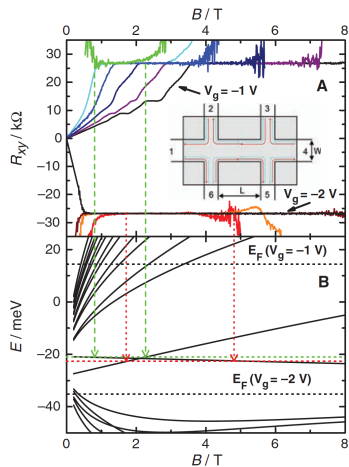


Figure: (a) Hall resistance, different fermi level via gate voltage (b) Fermi level versus landau energy

Further

Spin accumulation is still challenging task for experiment at that time. Eventually in 2012, German Molenkamp group (Würzburg uni) achieved it [10](ited by 118 times.). Theory suggested by Stanford plus Würzburg. Time limit and not gonna to be talked here.

Also, another subtle issue. It's actually only 'spin-like' Hall effect for its not spin at all but the Kramer pair (due to the strong mix by s-o coupling). Also note the argument of relationship with \mathbb{Z}_2 . In a topologically non-trivial system there must be odd number of Kramers' pairs crossing the Fermi energy. A general review can be seen at the annual review [11].

Matlab Code

Here for code.



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