5.5 Z_2 invariant : a simplified formula for insulators with space inversion symmetry

* Original derivation :

L. Fu and C. Kane, PRB 76, 045302 (2007)

* Proof of equivalence w/ the non-Abelian Berry connection formula :

R. Yu et al., PRB 84, 075119 (2011)

* Preliminaries :

(1) In the presence of TRS and SIS, energy bands are at least twofold degenerate for all $\vec{k}$.

Proof :

$$\left.\begin{aligned} \Pi\, h(\vec{k})\, \Pi^{-1} &= h(-\vec{k}) \\ \Theta\, h(\vec{k})\, \Theta^{-1} &= h(-\vec{k}) \end{aligned}\right\} \Rightarrow$$

$$\Pi\, h(\vec{k})\, \Pi^{-1} = \Theta\, h(\vec{k})\, \Theta^{-1}$$

$$\Rightarrow \quad h(\vec{k}) = \Pi\, \Theta\, h(\vec{k})\, \Theta^{-1}\, \Pi^{-1}$$

$\uparrow$

$\Pi^2 = \mathbb{1}$

$\Rightarrow \quad h(\vec{k})\, \Pi\Theta = \Pi\Theta\, h(\vec{k})$

$\Rightarrow \quad [\, h(\vec{k}),\, \Pi\Theta\,] = 0 \quad$ for all $\vec{k}$.

Suppose $\quad h(\vec{k})\, |u_{\vec{k}}\rangle = E_{\vec{k}}\, |u_{\vec{k}}\rangle$

Then,

$h(\vec{k})\left(\Pi\Theta\, |u_{\vec{k}}\rangle\right) =$

$= \Pi\Theta\; h(\vec{k})\, |u_{\vec{k}}\rangle = \Pi\Theta\; E_{\vec{k}}\, |u_{\vec{k}}\rangle$

$= \quad E_{\vec{k}}\left(\Pi\Theta\, |u_{\vec{k}}\rangle\right)$

$\Rightarrow \quad |u_{\vec{k}}\rangle$ and $\Pi\Theta\, |u_{\vec{k}}\rangle$ are eigenstates of $h(\vec{k})$ with the same eigenvalue $E_{\vec{k}}$.

Two possibilities:

(i) $|u_{\vec{k}}\rangle$ and $\pi\Theta|u_{\vec{k}}\rangle$ are the same state

(ii) $|u_{\vec{k}}\rangle$ and $\pi\Theta|u_{\vec{k}}\rangle$ are different states $\rightarrow$ 2 fold degeneracy at all $\vec{k}$.

For spin $\frac{1}{2}$ fermions, $\Theta^2 = -\mathbb{1}$, possibility (ii) is realized.

(2) At TRIM, eigenstates of $h(\vec{k})$ are also eigenstates of π.

Proof:

TRIM : $\vec{k}_{trim} \equiv \Gamma_i$

$$h(\Gamma_i) = \pi^{-1} h(\Gamma_i) \pi$$

$$\Rightarrow \quad [h(\Gamma_i), \pi] = 0 .$$

If $h(\Gamma_i)|\mu_{\Gamma_i}\rangle = E_{\Gamma_i}|\mu_{\Gamma_i}\rangle$,

then $\boxed{\pi|\mu_{\Gamma_i}\rangle = \zeta_{\Gamma_i}|\mu_{\Gamma_i}\rangle}$

$$\pi^2 = \mathbb{1} \Rightarrow \zeta_{\Gamma_i} = +1 \text{ or } -1$$

↑ parity eigenvalue

* Fu-Kane formula for $\mathbb{Z}_2$ invariant:

$$\boxed{(-1)^\nu = \prod_{i \in \text{TRIM}} \delta_i}$$

where $\boxed{\delta_i = \prod_{m=1}^{N} \xi_{2m}(\Gamma_i)}$

(2N occupied bands in the insulator)

$\xi_{2m}(\Gamma_i)$ = parity eigenvalue of $2m$-th occupied band at TRIM Γ_i.

$\nu = Z_2$ topological invariant

$$= \begin{cases} 0 \to \text{trivial insulator} \\ 1 \to \text{topological} \quad " \end{cases}$$

5.6 Bernevig - Hughes - Zhang model (BHZ)

* Theory:

B. A. Bernevig, T. L. Hughes and S. C. Zhang, Science 314, 1757 (2006).

* Experiment:

M. Konig et al., Science 318, 766 (2007).

* Motivation:

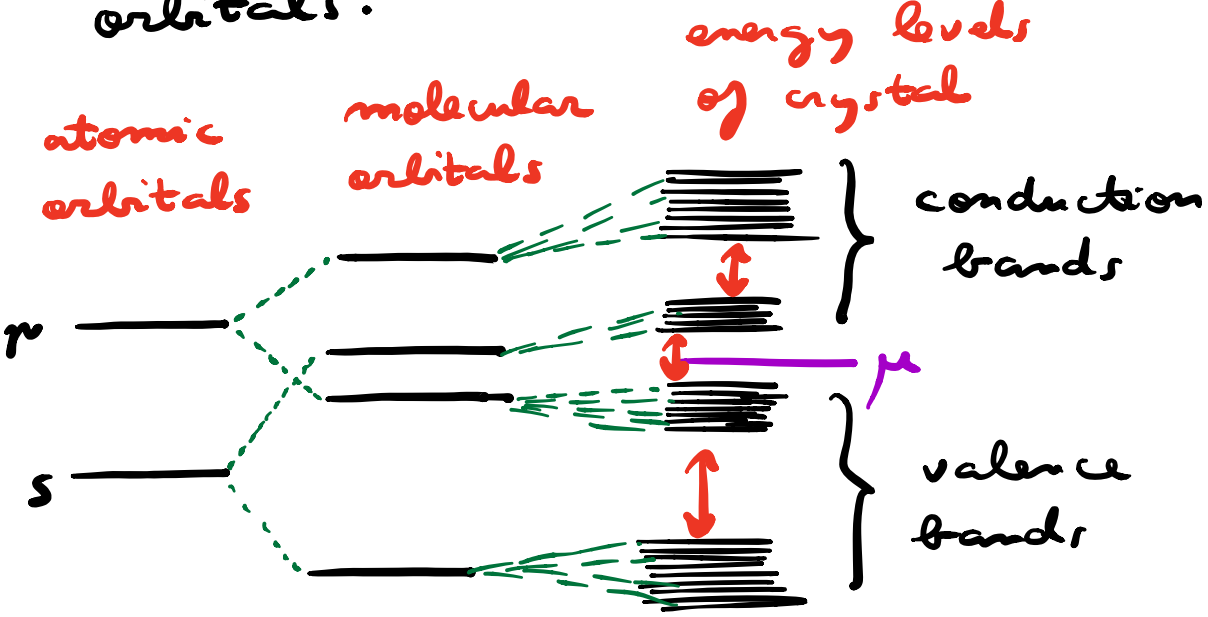
The spin-orbit-induced bandgap in graphene is too small (~ 100 mK)

Can one find another system with larger gap?

Guiding principle: band inversion.

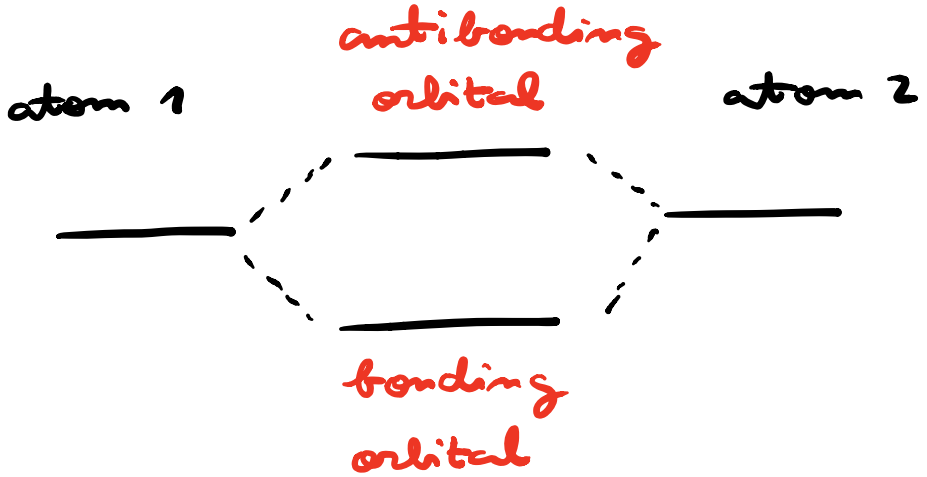
* Low-energy electronic structure in typical semiconductors:

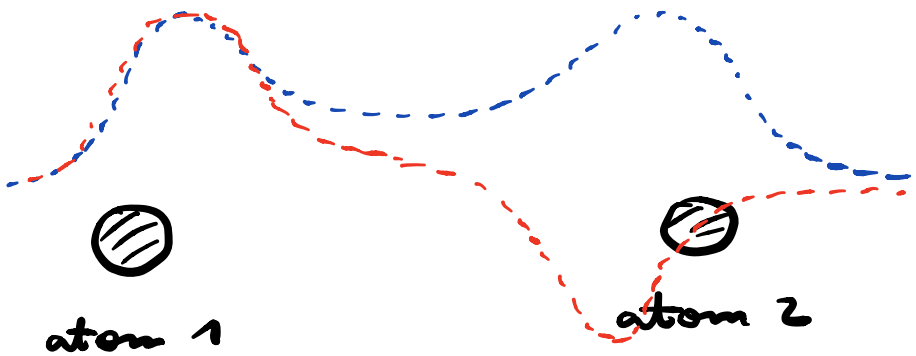
valence e^--s occupy s and p orbitals.



↕ = energy gap

Molecular orbitals : hybridised orbitals of 2 atoms.





— bonding

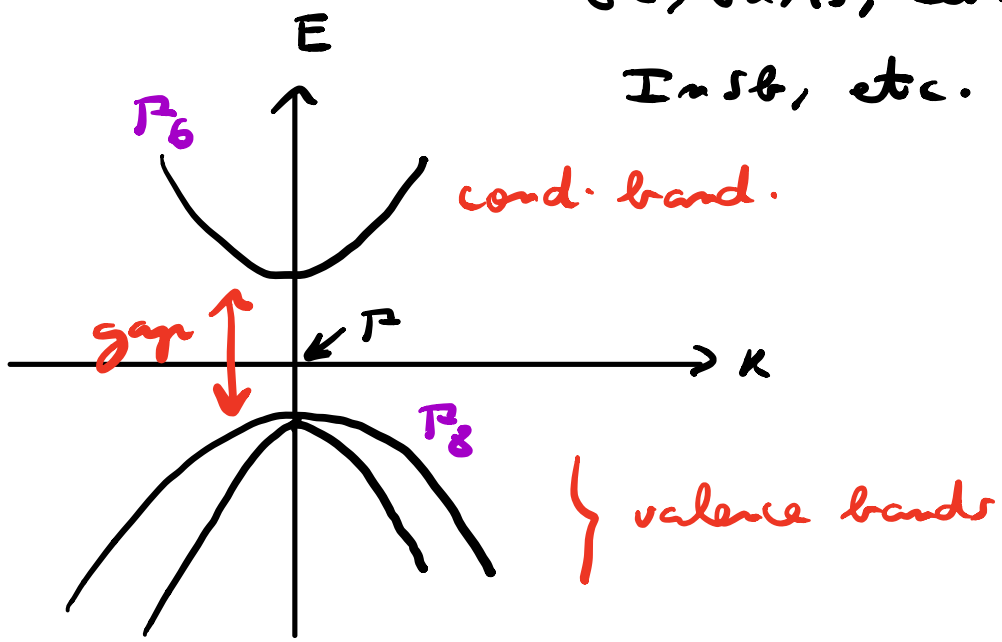
— antibonding

bonding and antibonding orbitals have opposite parities under inversion.

The electronic structure of ordinary semiconductors is adiabatically connected to molecular orbitals (decoupled molecules)

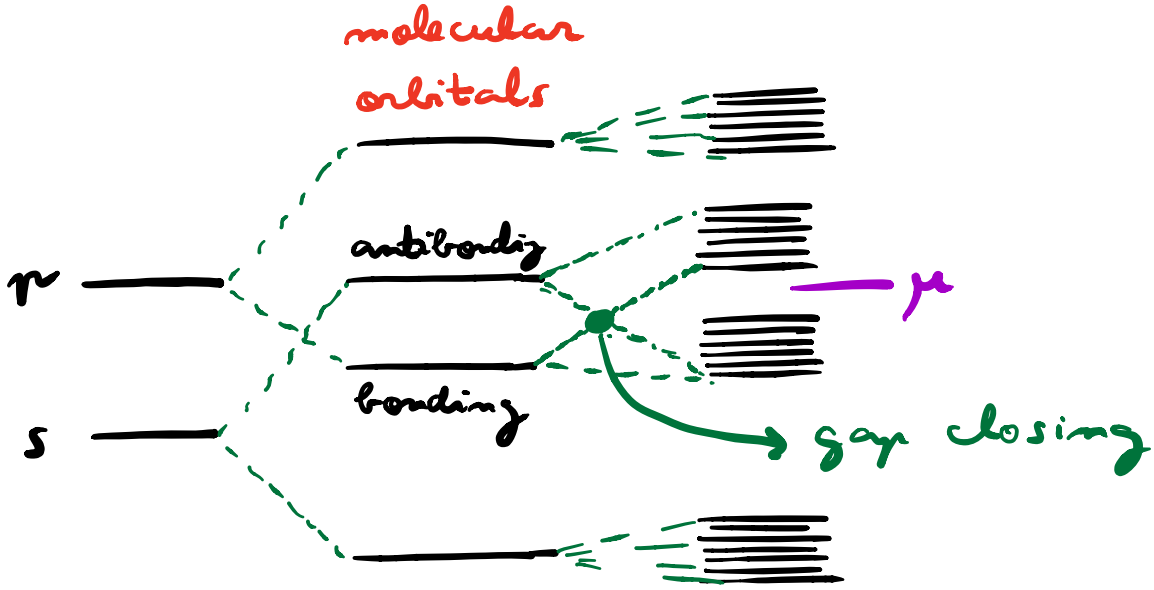
$\Rightarrow$ topologically trivial.

Ge, GaAs, CdTe, InSb, etc.



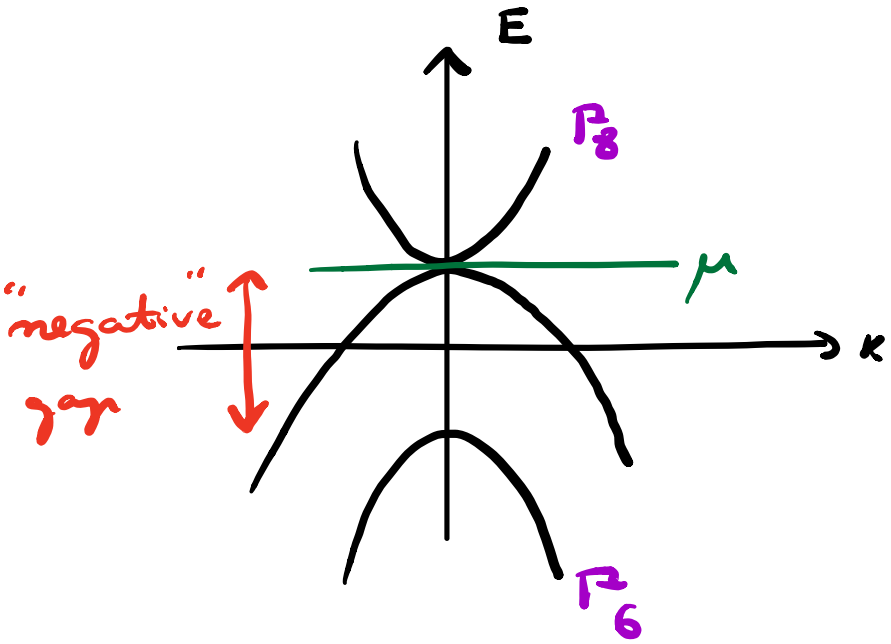
Γ_8 is below Γ_6.

* Semiconductors with inverted bands



This electronic structure is not adiabatically connected to molecular orbitals ⇒ topologically nontrivial?

Only one example: HgTe

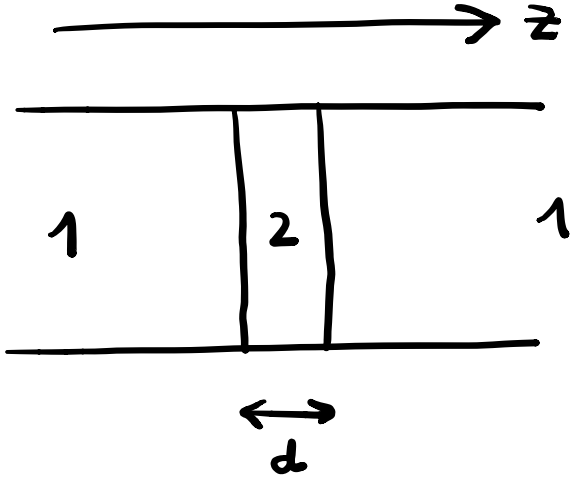


Γ_6 is below Γ_8. Inverted bands.

Problem: HgTe is not an insulator

Yu and Cardona, "Principles of Semiconductors"

* In order to coax HgTe into being an insulator, BHZ proposed to confine HgTe into a "quantum well" (QW)



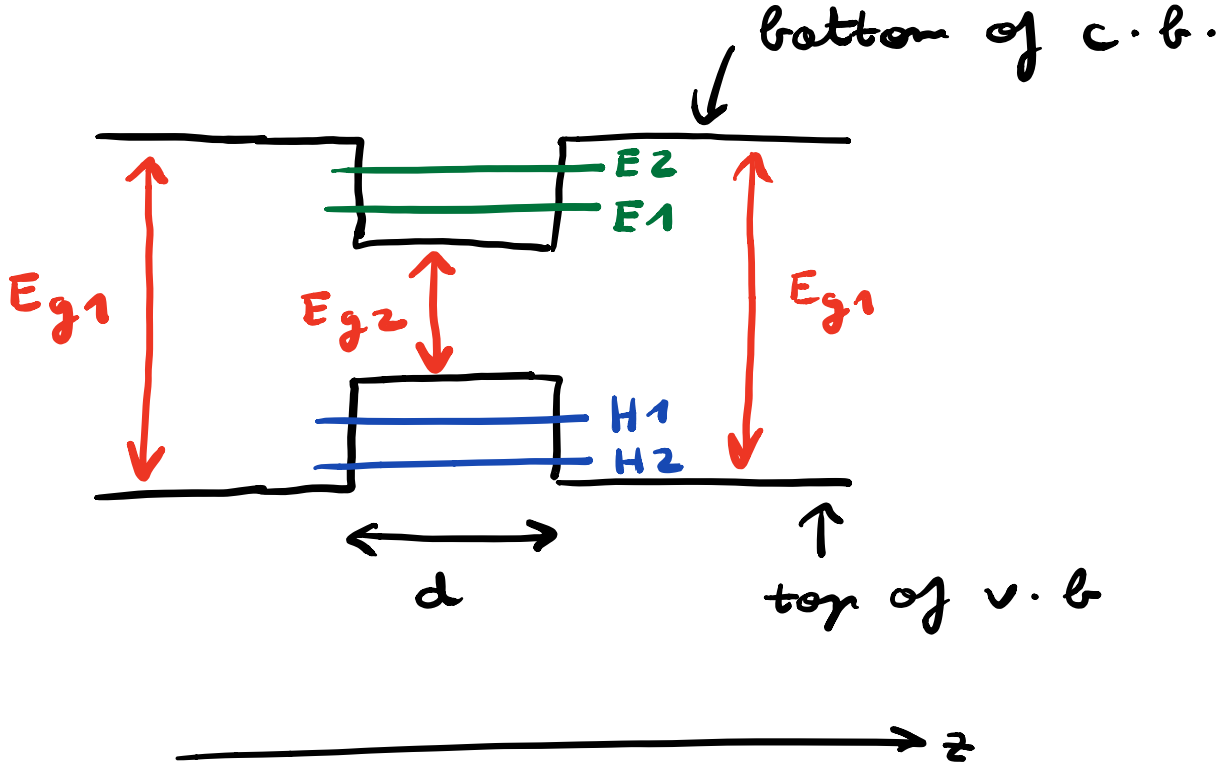
1 : CdTe ("ordinary" semiconductor)

2 : HgTe

d = thickness of QW

translational symmetry in xy plane.

Bottom of conduction band and top of valence band at $k = 0$:



E1, E2, ... : quantum well states in c.b.

H1, H2, ... : quantum well states in v.b.

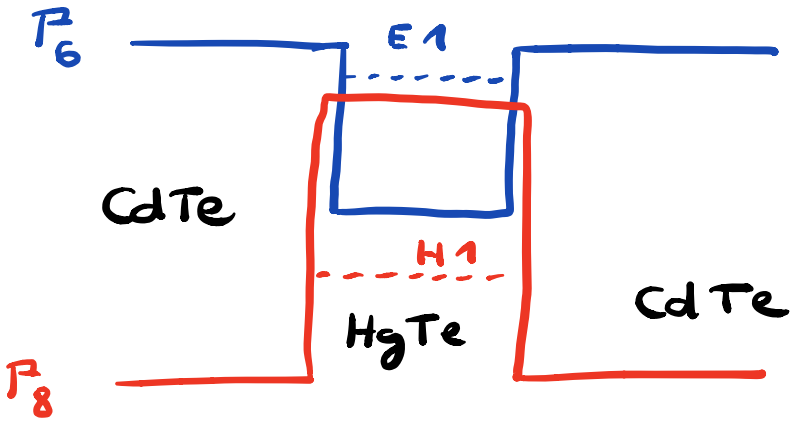
Confinement energy of QWS

$$\sim \frac{\hbar^2}{2 m_{eff}} \frac{1}{d^2}$$

For small d, only E1 and H1 matter for low-energy properties.

In this regime, the QW is effectively 2D (in xy plane).

* Prediction of BHZ



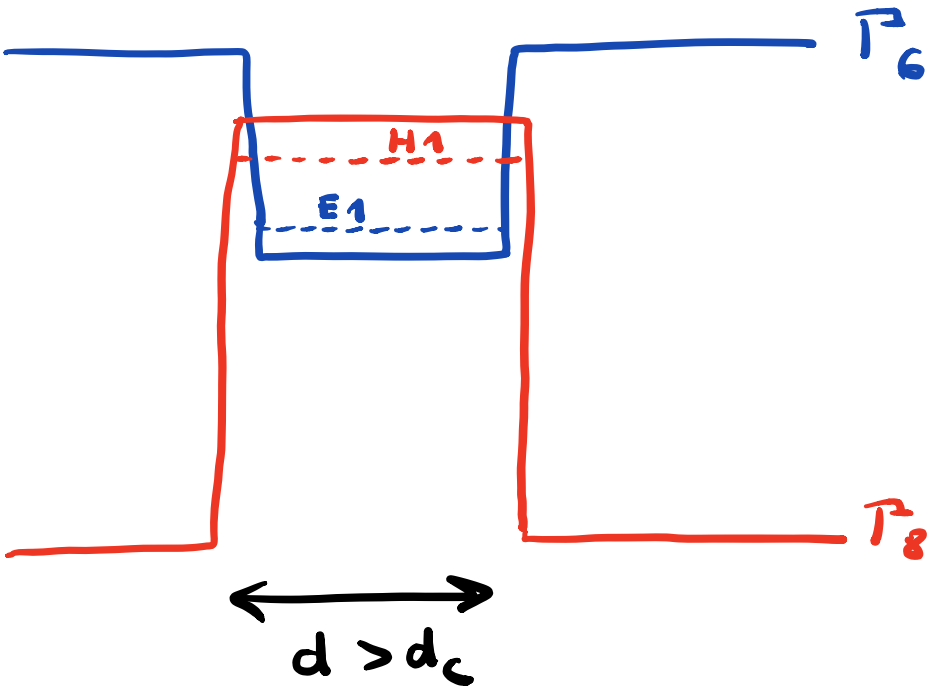
$d < d_c$ ← critical thickness

E1 > H1 in HgTe

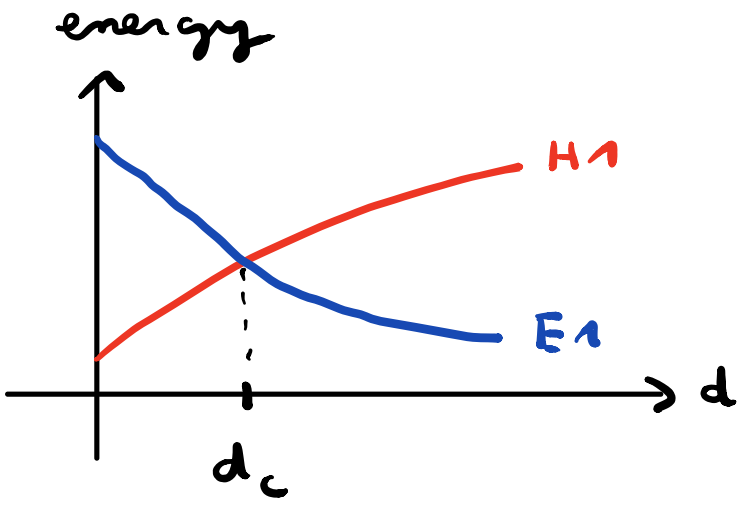
→ normal ordering

→ trivial insulator

Increase thickness:



E1 < H1 → inverted ordering → topological insulator.



$d_c = 6.3$ nm

Band inversion at $d = d_c$.

→ topological phase transition.

* Effective Hamiltonian for E1 and H1 quantum well states.

Assume SIS in the xy plane.

⟶ TRS + SIS give

twofold degenerate bands.

$\Rightarrow$ basis for low-energy states:

$$\{ |E1+\rangle, |E1-\rangle, |H1+\rangle, |H1-\rangle \}$$

where + and - are partners by time-reversal.

These basis states are eigenstates of k_{eff} at $\vec{k} = 0$, by construction.

$|E\rangle$ and $|H\rangle$ are parity eigenstates:

$$\pi |E\rangle = |E\rangle$$

$$\pi |H\rangle = -|H\rangle$$

$|E\rangle$ and $|H\rangle$ have opposite parity because they come from bonding and antibonding molecular orbitals, respectively.

What is $\underbrace{h_{eff}(\vec{k})}$ at $\vec{k} \neq 0$?

↑

4×4 matrix

The form of matrix elements can be established from symmetry.

$\langle E1, \pm | h_{eff}(\vec{k}) | H1, \pm \rangle$

has to be odd in $\vec{k}$

because E1 and H1 have opposite parities.

To lowest order, the matrix element is linear in $\vec{k}$.

$$\langle E1, \pm | h_{eff}(\vec{k}) | E1, \pm \rangle$$

and $\langle H1, \pm | h_{eff}(\vec{k}) | H1, \pm \rangle$

are even functions of $\vec{k}$.

It turns out that

$|H1, +\rangle$ is formed from

atomic orbitals of type

$$| \underline{p_x + i p_y}, \uparrow \rangle$$

l, m_l

$\uparrow$ spin

s, m_s

$$\Rightarrow \quad j_z = 1 + \frac{1}{2} = \frac{3}{2}$$

$|E\uparrow, +\rangle$ is formed from atomic orbitals of type $|s, \uparrow\rangle$

$$\Rightarrow j_z = 0 + \frac{1}{2} = \frac{1}{2}$$

If we require that $h_{eff}(\vec{k})$ be rotationally symmetric in the (k_x, k_y) plane,

← reasonable for a continuum model.

$$\langle E\uparrow, + | h_{eff}(\vec{k}) | H\uparrow, +\rangle$$

$$\sim k_x + i k_y$$

↑ provides $\Delta j_z = 1$