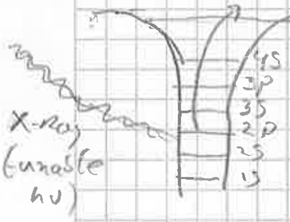
X-ray absorption spectroscopy (XAS)



2p energy for 3d TM : 400 - 1000 eV

Dipole selection rules : $\Delta \ell = +/- 1$ $\Delta S = 0$

From s-state $\rightarrow$ unoccupied p DOS

From p $\rightarrow$ d unoccupied ~~d~~ DOS

Fermi golden rule : $W_{fi} \propto |\langle \psi_f | T_i | \psi_i \rangle|^2 \, \delta(E_f - E_i - h\nu)$

role
only from occupied
transition matrix

Dipole transitions : $W_{fi} \propto |\langle \psi_f | \hat{E}_q \cdot \vec{r} | \psi_i \rangle|^2 \, \delta$. (lifetime + exp. broadening)

E-field of $h\nu$ e^- position

* 2p $\rightarrow$ 3d transitions : overlap of 2p core hole with 3d DOS

$\longrightarrow$ interactions, change of ψ_i and 3d DOS

Incorporated in (atomic) multiplet theory :

$\Longrightarrow$ Identification of valence state + orbital occupancy
+ crystal field splitting

XMCD : $q = +/- 1$ $\hat{\varepsilon}_{\pm 1} = \mp \frac{1}{\sqrt{2}} (\hat{x} \pm i \hat{y})$ $(\hat{\varepsilon}_0 = \hat{z})$

"dipole rule" : $\Delta m_j = q$ (in spherical harmonics)

dichroism : $\frac{I_+ - I_-}{I_+ + I_-} \propto \langle L_z \rangle \neq 0$ for Ferro-, Ferri-, Altermagnets

* Jahn-Teller Effect
* Charge transfer Insulators

Topological insulators

Topology : - distinction of classes that are same under continuous/adiabatic transformations. (Homeomorphic)

- Transition between classes only through singularity (or break time-reversal symmetry)

Example: Möbius strip vs "normal" band : 1 surface, 1 edge, $\varphi = 4\pi$
$\hookrightarrow$ 2 surfaces, 2 edges, $\varphi = 2\pi$

* Euler characteristic : $V - E + F = \chi$ $\chi = 2 - 2g$ (genus # of holes)

vertices (corners)   edges   faces   2 sphere 0 torus

Football : Pentagons + Hexagons $V - E + F = \frac{5P - 6H}{3} - \frac{5P - 6H}{2} + P + H = \frac{P}{6} (= 2)$

$\Longrightarrow$ always 12 pentagons χ : topological invariant.

* $\mathbb{Z}_2$ topological invariants : Königsberg bridge problem

$\nu = 0$ Euler route possible (trivial, Paris)

Odd number of bridges from region $\longrightarrow$ $\nu = 1$ Euler route not possible (non-trivial)

$\mathbb{Z}_2$ in bandstructures

(Easy approach only for inversion symmetric crystal structure

- Consider parity of state: (anti)bonding, even/odd, (anti)symmetric
  + or −
- Odd number of parity inversions throughout 3D B.Z.: ν
  Even (or zero) $\Longrightarrow \nu = 0$

Formalise: [Relevance of inversion symmetry]

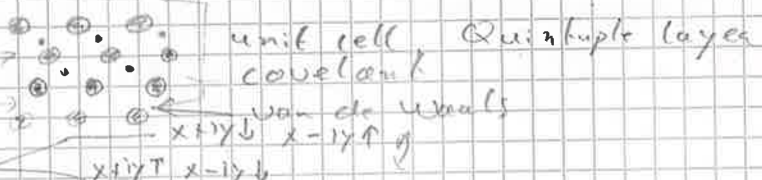
- 8 time-reversal invariant momenta (TRIM) in 3D B.Z
  4 in 2D B.Z. $+k = -k \rightarrow$ half-way between Γ points

others equivalent by symmetry

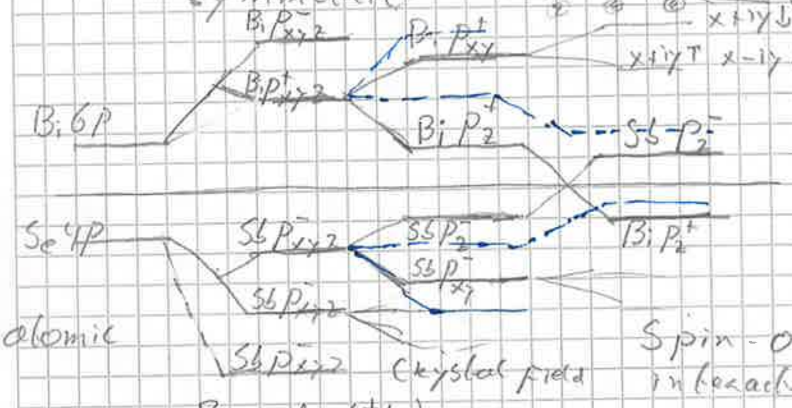
$i = 1, \ldots, 8 \quad \delta_i = \prod_{m=1}^{N} \xi_{i,2m}$ parity of state 2m at TRIM i

$(-1)^\nu = \prod_{i=1}^{8} \delta_i$ parity from TB or DFT

Example: Bi_2Se_3



Inversion symmetric

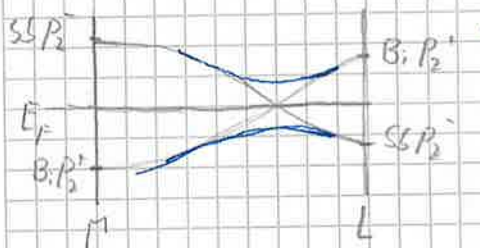


Γ - point
L - point (similar for Z, and F)

Bonds (+/−)

[Slide]

Band structure from Γ → L (Z, F)



— avoided crossing due to SOI

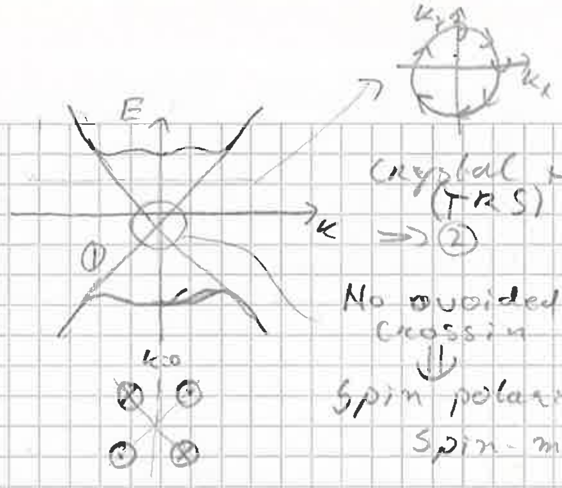
SOI causes band inversion
+ opens gap around E_F
$\Longrightarrow$ insulator

Consequences: At interface $\nu = 1 \rightarrow \nu = 0$ (vacuum)
Singularity → state must exist: topological protection

- Time reversal symmetry in k-space $E(\vec{k}, \uparrow) = E(-\vec{k}, \downarrow)$
  at TRIM: $\vec{k} = 0$ or $\vec{k} = \frac{1}{2}\vec{G} \Longrightarrow E(\uparrow) = E(\downarrow)$ degenerate

How to realise protected state?

(1st)



crystal + (TRS) ⟹ ②

No avoided crossin

⇓

Spin polarised

— continuous dispersion can avoid state

— State guaranteed in gap

Spin polarised

Spin-momentum locking + Dirac cone

[Topological protection]

hybridisation change # of available states

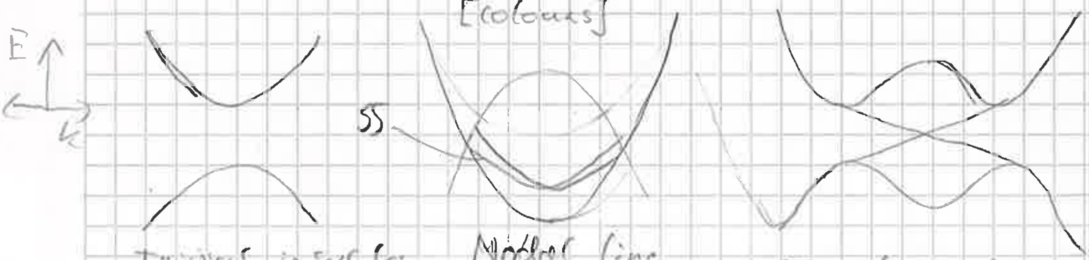
Shockley Edge states (1938):

Closing + reopening of bandgap (projected) ⟹ Edge state

1 state (↑) per reopening and edge / surface

→ count # of crossings in 3D BZ ⟹ topology?

[colours]



Trivial insulator semiconductor

Nodal line (semi) metal (small SOI)

Topological Insulator (larger SOI)

- Local gap + SS
- Crystal symmetry can protect band crossings
  ⟹ Topological crystalline insulator
- Dirac SM