LECTURE 14

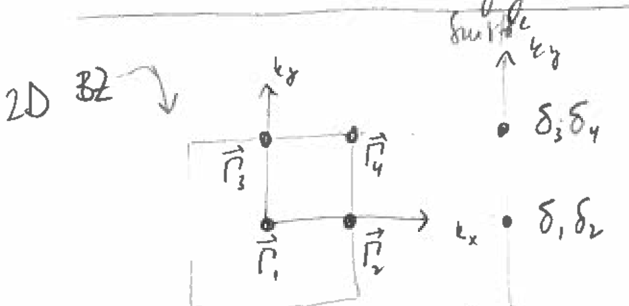
Topological Insulators in 3D

- Moore & Balents, PRB **75**, 121306 (2007)
- R. Roy, PRB **79**, 195322 (2009); arXiv:0607531
- Fu, Kane & Mele, PRL **98**, 106803 (2007)

Topological classification of 3D, T-invariant insulators

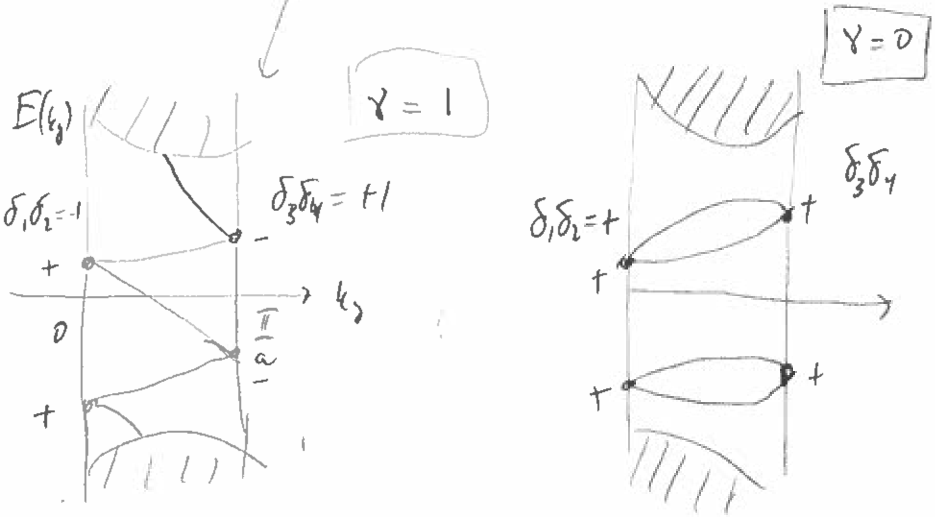
Result: In 3D there exist 16 classes of insulators labeled by 4 $\mathbb{Z}_2$ indices $(\nu_0; \nu_1 \nu_2 \nu_3)$.

Work in analogy to 2D:



$$\delta_i = \frac{\sqrt{\det[w(\vec{\Gamma}_i)]}}{\mathrm{Pf}[w(\vec{\Gamma}_i)]} \overset{P}{=} \prod_{m \in occ.} \xi_{2m}(\vec{\Gamma}_i)$$

$$(-1)^\nu = \prod_{i=1}^{4} \delta_i$$

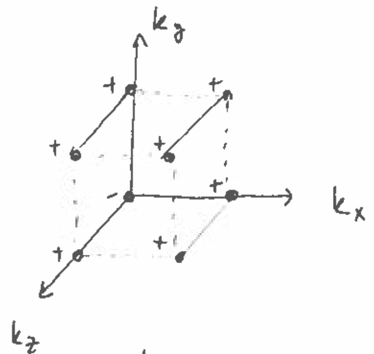


$\mathbb{Z}_2$ classification in 3D

$\vec{\Gamma}_i = -\vec{\Gamma}_i + \vec{G}$

Define 8 TRIM $\quad \vec{\Gamma}_{i=(n_1 n_2 n_3)} = \frac{1}{2}\left(n_1 \vec{b}_1 + n_2 \vec{b}_2 + n_3 \vec{b}_3\right) \quad , \quad n_j = 0, 1$

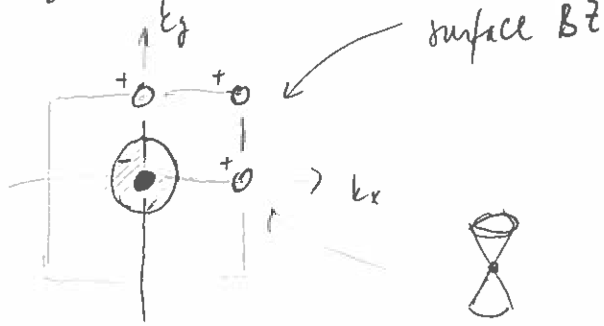
$\vec{b}_j$ - primitive vectors of the Rec. lattice.



Define δ_i's for each $\vec{\Gamma}_i$ as before.

$$\delta_i = \frac{\sqrt{\det[w(\vec{\Gamma}_i)]}}{Pf[w(\vec{\Gamma}_i)]} \overset{P}{=} \prod_{m \in occ.} \xi_{2m}(\vec{\Gamma}_i)$$

- only a product of 4 δ_i's in the same plane is gauge invariant!



Surface states on $z=0$ plane.

At surface TRIM, states must be doubly degenerate due to the Kramers theorem. $\Rightarrow$ 2D Dirac cones

- When the sign changes there is an odd # of fermi crossings between the TRIMs, (otherwise the # is even, possibly 0).

Show fig 2, Fu, Kane, Mele PRL

Strong & weak indices.

Out of 8 δ_i's one can define 4 $\mathbb{Z}_2$ invariants

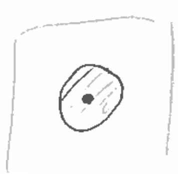
$$(-1)^{\nu_0} = \prod_{n_j=0,1} \delta_{n_1 n_2 n_3} \qquad 1 \text{ "strong invariant"}$$

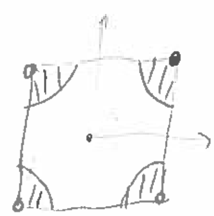
$$(-1)^{\nu_i} = \prod_{\substack{n_i=1 \\ n_{j\neq i}=0,1}} \delta_{n_1 n_2 n_3} \qquad 3 \text{ "weak invariants"}$$

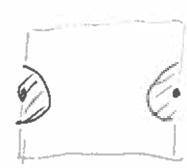
$\nu_0 = 1$ "Strong topological insulator" (STI)

- has ODD number of Dirac states on all crystal surfaces.
- Projection of $\vec{g} = \nu_1 \vec{b}_1 + \nu_2 \vec{b}_2 + \nu_3 \vec{b}_3$ onto the surface BZ determines the position of the Dirac point (if there is only one)

Example: (1;000) (1;111) (1,100)







Bi_2Se_3
Bi_2Te_3
⋮

Bi_xSb_{1-x}
(5 dirac points)

?

$\underline{\nu_0 = 0}$ — "Weak TI" if $\nu_i \neq 0$ for some i

Trivial if $\nu_i = 0$.

- in this case we have even # of Dirac points on surfaces, possibly 0.

Show some ARPES data.