TOPOLOGICAL BAND THEORY IN THREE DIMENSIONS

③ $\mathbb{Z}_2$ topological insulators

Generalisation of the quantum spin Hall insulator to 3D crystals with time-reversal symmetry.

Fu, Kane and Mele, PRL 98, 106805 (2007)
Moore and Balents, PRB 79, 195322 (2009)
Roy, PRB 79 195322 (2009)

3.1 Reminder: $\mathbb{Z}_2$ invariant in 2D

For simplicity, assume crystal with inversion symmetry

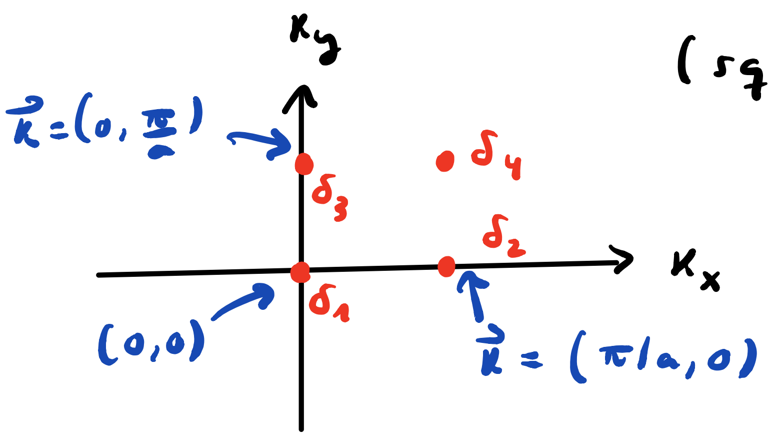
space

* Fu-Kane formula for $\mathbb{Z}/_2$ invariant (lec 22):

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

$i \in \{\text{TRIMs}\}$

$\delta_i = \pm 1$



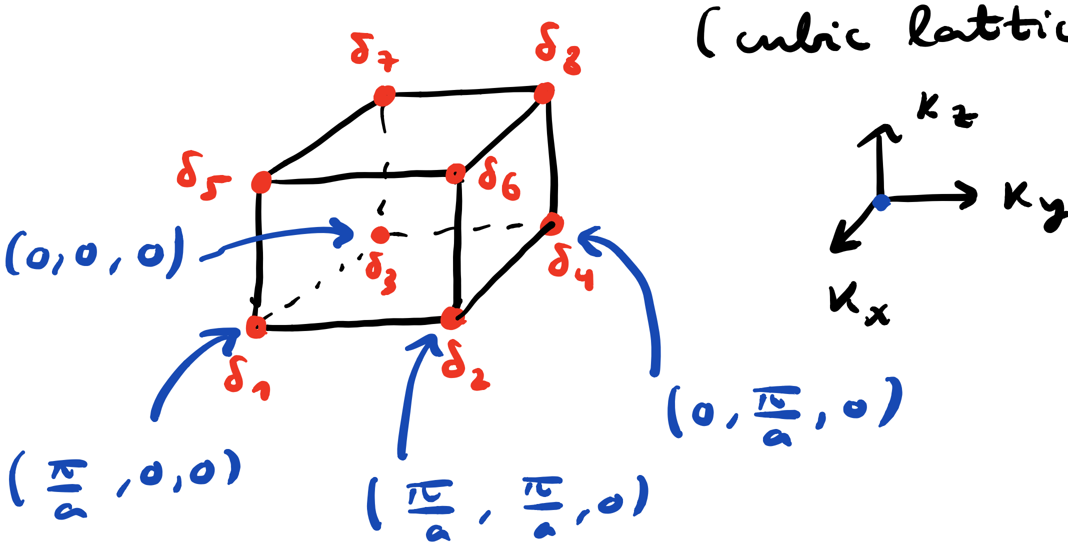
(sq. lattice)

$$\nu = \begin{cases} 0 \rightarrow \text{trivial} \\ 1 \rightarrow \text{topologically nontrivial} \end{cases}$$

3.2 $\mathbb{Z}_2$ invariants in 3D

We can't make 3D Chern #s out of 2D, but we can make 3D $\mathbb{Z}_2$ invariants out of 2D.

(cubic lattice)



$$(-1)^{\nu_0} = \prod_{i=1}^{8} \delta_i$$

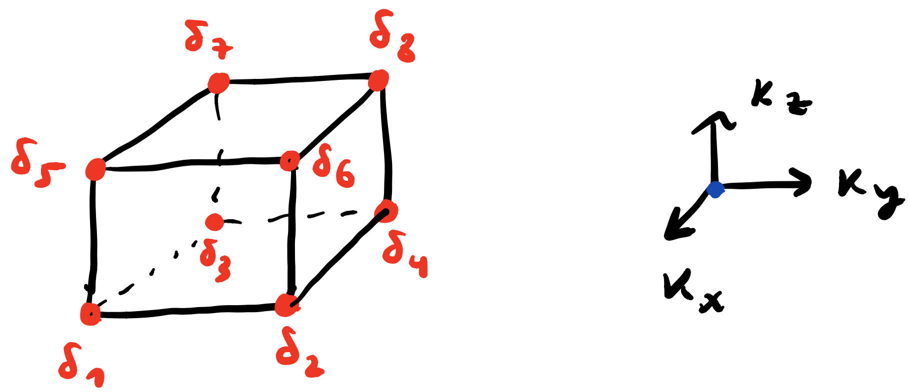
$$\nu_0 = \begin{cases} 0 \to \text{trivial} \\ 1 \to \text{topological} \end{cases}$$

?

This is a good guess, but it turns out that the situation is richer. For example, an insulator can be topologically nontrivial even when $\nu_0 = 0$. Regardless, $\nu_0 = 1$ is always topological.

In 3D, there's more than one $\mathbb{Z}/2$ invariant. Each plane of the cube above is invariant under time-reversal $\rightarrow$ we can define a $\mathbb{Z}/2$ invariant for each plane.

6 faces of the cube $\rightarrow$ 6 $\mathbb{Z}/2$ invariants.



$$(-1)^{\nu_1} = \delta_1 \delta_2 \delta_5 \delta_6$$

$$(-1)^{\nu_2} = \delta_2 \delta_4 \delta_6 \delta_8$$

$$(-1)^{\nu_3} = \delta_5 \delta_6 \delta_7 \delta_8$$

$$(-1)^{\nu_1'} = \delta_3 \delta_4 \delta_7 \delta_8$$

$$(-1)^{\nu_2'} = \delta_1 \delta_3 \delta_5 \delta_7$$

$$(-1)^{\nu_3'} = \delta_1 \delta_2 \delta_3 \delta_4 \qquad \delta_i \in \{\pm 1\}$$

$$\nu_i \in \{0, 1\} \qquad (\mathrm{mod}\ 2)$$

$$\nu_i' \in \{0, 1\}$$

But, these invariants are not all independent from one another.

Constraints:

$$(-1)^{\nu_1}(-1)^{\nu_1'} = (-1)^{\nu_2}(-1)^{\nu_2'}$$
$$= (-1)^{\nu_3}(-1)^{\nu_3'}$$

i.e.,

$$\nu_1 + \nu_1' = \nu_2 + \nu_2' \pmod 2$$
$$\nu_2 + \nu_2' = \nu_3 + \nu_3' \quad (\quad '' \quad)$$

(2 constraints)

$6 - 2 = 4$ independent $\mathbb{Z}/_2$ invariants.

By convention, we write them as

$$(\nu_0 ; \nu_1 , \nu_2 , \nu_3)$$

where
$$\begin{aligned} \nu_0 &= \nu_1 + \nu_1' \\ &= \nu_2 + \nu_2' \\ &= \nu_3 + \nu_3' \end{aligned}$$

ν_0 : "strong" topological invariant

ν_1, ν_2, ν_3 : "weak" topological invariants.

If $\nu_0 = 1$, the insulator is certainly topological.

If $\nu_0 = 0$, the insulator can still be topological (in a slightly different sense to be discussed later) provided that $(\nu_1, \nu_2, \nu_3) \neq (0,0,0)$.

If $(\nu_0 ; \nu_1, \nu_2, \nu_3) = (0 ; 0, 0, 0)$, then the insulator is topologically trivial.

* General formula for $\mathbb{Z}/2$ invariants in 3D crystals (not necessarily cubic) with inversion symmetry:

TRIM:

$$\Gamma_{i=(n_1,n_2,n_3)} =$$

$$= \frac{1}{2} \left(n_1 \vec{b}_1 + n_2 \vec{b}_2 + n_3 \vec{b}_3 \right)$$

where $n_j = 0, 1$

and $\vec{b}_i$ are reciprocal lattice vectors defining the 1BZ.

Cubic lattice:

$$\vec{b}_1 = \frac{2\pi}{a} (1, 0, 0)$$

$$\vec{b}_2 = \frac{2\pi}{a} (0, 1, 0)$$

$$\vec{b}_3 = \frac{2\pi}{a} (0, 0, 1)$$

$$(-1)^{\nu_0} = \prod_{n_1, n_2, n_3} \delta_{(n_1, n_2, n_3)}$$

$$(-1)^{\nu_1} = \prod_{n_2, n_3} \delta_{(1, n_2, n_3)}$$

$$(-1)^{\nu_2} = \prod_{n_1, n_3} \delta_{(n_1, 1, n_3)}$$

$$(-1)^{\nu_3} = \prod_{n_1, n_2} \delta_{(n_1, n_2, 1)}$$

ν_0 is a genuinely 3D invariant (not associated to a single plane);

ν_1, ν_2, ν_3 : $\mathbb{Z}_2$ invariants for different 2D planes