2. 3D Topological insulator

let's consider the low-energy continuum model for prototypical 3D topological insulators such as Bi_2Se_3. The bulk electronic structure of Bi_2Se_3 near the Fermi level is described by two p-orbitals $P1_z^+$ and $P2_z^-$ with $\pm$ denoting parity. Defining the basis $\{ |P1_z^+, \uparrow\rangle, |P1_z^+, \downarrow\rangle, \cancel{|P2_z} |P2_z^-, \uparrow\rangle, |P2_z^-, \downarrow\rangle \}$ and ~~remaind~~ retaining the wave vector $\vec{k}$ up to quadratic order, the low-energy effective Hamiltonian around the Γ point is given by:

$$H_{eff}(\vec{k}) = \begin{bmatrix} -M(\vec{k}) & 0 & A_1 k_z & A_2 k_- \\ 0 & M(\vec{k}) & A_2 k_+ & -A_1 k_z \\ A_1 k_z & A_2 k_- & -M(\vec{k}) & 0 \\ A_2 k_+ & -A_1 k_z & 0 & -M(\vec{k}) \end{bmatrix}$$

$$= A_2 k_x \alpha_1 + A_2 k_y \alpha_2 + A_1 k_z \alpha_3 + M(\vec{k}) \cdot \alpha_4$$

where $k_\pm = k_x \pm i k_y$ and $M(\vec{k}) = m_0 - B_1 k_z^2 - B_2 (k_x^2 + k_y^2)$. The 4×4 matrics α_μ are given by the Dirac representation:

$$\alpha_j = \begin{bmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{bmatrix}, \quad \alpha_4 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Next, let's consider the lattice model of above Hamiltonian, which can calculate the $\mathbb{Z}_2$ invariant identifying whether a phase is topological nontrivial or trivial.

The simplest 3D lattice is the cubic lattice. We make the changes as following (ignore lattice constant a).

$$\begin{cases} k_i \rightarrow \sin k_i \\ k_i^2 \rightarrow 2(1-\cos k_i) \end{cases}$$

and simplify the coefficients to obtain the isotropic lattice Hamiltonian:

$$H_{eff}(\vec{k}) = A(\alpha_1 \sin k_x + \alpha_2 \sin k_y + \alpha_3 \sin k_z) + \left[m_0 + r\sum_i (1-\cos k_i)\right]\alpha_4$$

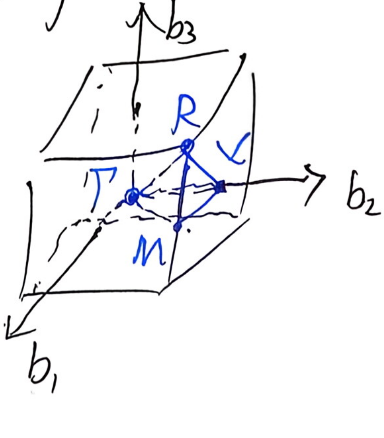
where we difine $A = A_1 = A_2$ and $r = -2B_1 = -2B_2$.

Then, we use Fu-Kane method to ~~cout~~ calculate the Z_2 topological invariant for this system:

$$(-1)^{\nu} = \prod_{i=1}^{N_{TRIM}} \mathrm{sgn}[M(\Lambda_i)]$$

In this 3D cubic lattice, there are 8 TRIM (Time-Reversal Invariant Momenta which are invariant under $k_i \rightarrow -k_i$) point:

$$\begin{cases} \Gamma: (0,0,0) \\ X: (\pi,0,0) / (0,\pi,0) / (0,0,\pi) \\ M: (\pi,\pi,0) / (\pi,0,\pi) / (0,\pi,\pi) \\ R: (\pi,\pi,\pi) \end{cases}$$



The ~~m~~ mass term is:

$$M(\vec{k}) = m_0 + r\sum_{i=x,y,z}(1-\cos k_i)$$

so we can calculate the mass term for each group of point:

$$\begin{cases} \Gamma: M = m_0 \\ X: M = m_0 + 2r \\ M: M = m_0 + 4r \\ R: M = m_0 + 6r. \end{cases}$$

Now we subsitute these mass terms into the $\mathbb{Z}_2$ topologycal invariant formula

$$(-1)^{\nu} = \mathrm{sgn}(m_0) \times \mathrm{sgn}(m_0+2r)^3 \times \mathrm{sgn}(m_0+4r)^3 \times \mathrm{sgn}(m_0+6r)$$

$$= \mathrm{sgn}(m_0) \times \mathrm{sgn}(m_0+2r) \times \mathrm{sgn}(m_0+4r) \times \mathrm{sgn}(m_0+6r)$$

$$= \begin{cases} -1 \quad \left(0 > \frac{m_0}{r} > -2,\ -4 > \frac{m_0}{r} > -6\right) \\ 1 \quad \left(\frac{m_0}{r} > 0,\ -2 > \frac{m_0}{r} > -4,\ -6 > \frac{m_0}{r}\right) \end{cases}$$

let's return to the continuum isotropic Hamiltonian to obtain the θ term. Consider the Hamiltonian around the Γ point ~~can be~~ simplified by ignoring the terms second-order in k_i:

$$H_{TI}(\vec{k}) = A\vec{k}\cdot\vec{\alpha} + m_0\alpha_4$$