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 $\{|P1_z^+,\uparrow\rangle, |P1_z^+,\downarrow\rangle, |P2_z^-,\uparrow\rangle, |P2_z^-,\downarrow\rangle\}$ 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).

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

and simplify the coefficients to obtain the isotropic lattice Hamiltonian:

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

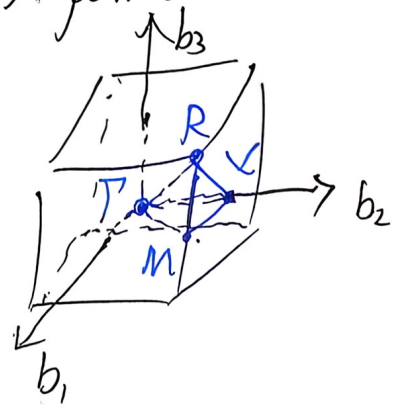
where we difine $A = A_1 = A_2$ and $\gamma = -2B_1 = -2B_2$.

Then, we use Fu-Kane method to ~~cal~~ calculate the $\mathbb{Z}_2$ 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 $k_i \to -k_i$) 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

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

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

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

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:

$$H_{TI}(\vec{k}) = A\vec{k}\cdot\vec{\Sigma} + m_0\Sigma_4$$

Because this Hamiltonian describes a topological insulator, m_0 is less than zero $((-1)^{\nu} = \mathrm{sgn}(m_0))$. Except for the negative mass m_0, this is the usual Dirac Hamiltonian $(\hbar\vec{k} \to c\vec{p})$.

In the presence of an external electromagnetic vector potential $\vec{A}$, minimal coupling results in: $\vec{p}$

$$\vec{p} \to \cancel{\vec{p} \pm e\vec{A}} \quad \vec{p} - (-e)\vec{A} = \vec{p} + e\vec{A}$$

where $e > 0$ being the magnitude of the electron charge.

At the same time, because of the external electromagnetic scalar potential A_0, the energy density is modified as:

$$\psi^{\dagger} H_0 \psi \to \psi^{\dagger}(H_0 - eA_0)\psi$$

So the action of the system in the presence of an external electromagnetic four potential $A_\mu = (A_0, -\vec{A})$ is written in the follow relativistic form;

$$S_{TI} = \int dt d^3x \, \psi^{\dagger} \{ i(\partial_t - ieA_0) - [H_{TI}(\vec{k} + e\vec{A})] \} \psi$$

$$= \int dt d^3x \, \psi^{\dagger} [i(\partial_t - ieA_0) - \overset{(-i\nabla + e\vec{A})\vec{\alpha}}{\cancel{(-i\nabla)\vec{\alpha}}} - m_0 \alpha_4] \psi$$

where $\psi^{\dagger}(\vec{x}, t)$ is a fermionic field representing the basis of the Hamiltonian.

Then we need to convert from the basis of $\psi^\dagger$ and α_j matrix to the relativistic ~~form~~ basis of $\bar{\psi}$ and γ matrices:

$$\begin{cases} \gamma^0 = \alpha_4 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\ \gamma^j = \alpha_4 \alpha_j = \begin{bmatrix} 0 & \sigma_j \\ -\sigma_j & 0 \end{bmatrix} \\ \gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \\ \bar{\psi} = \psi^\dagger \gamma^0 \end{cases}$$

To introduce $\bar{\psi}$, ~~wl~~ we use the identity $(\gamma^0)^2 = \mathbb{I}_{4\times4}$, so the ~~action~~ Lagrangian be rewritten as:

$$\begin{aligned} \cancel{S_{TI}}\, \mathcal{L}_{TI} &= \bar{\psi}\gamma^0[i(\partial_t - ieA_0) + i\nabla\vec{\alpha} - e\vec{A}\vec{\alpha} - m_0\alpha_4]\psi \\ &= \bar{\psi}\left[\gamma^0(i\partial_t + i\nabla\vec{\alpha}) + \gamma^0(eA_0 - e\vec{A}\vec{\alpha}) - m_0\gamma^0\alpha_4\right]\psi \\ &= \bar{\psi}\left[i(\gamma^0\partial_t + \nabla\cdot\vec{\gamma}) + (eA_0\gamma^0 - e\vec{A}\vec{\gamma}) - m_0\right]\psi \\ &= \bar{\psi}(i\gamma^\mu\partial_\mu + e\gamma^\mu A_\mu - m_0)\psi \\ &= \bar{\psi}[i\gamma^\mu(\partial_\mu - ieA_\mu) - m_0]\psi \end{aligned}$$

In order to be convenient to study the system, we transform the system from Mikowski spacetime to Euclidean spacetime:

$$S_{TI}^E = -iS_{TI}.$$

We rewrite t, A_0 and γ^j as following:

$$\begin{cases} t \to i\tau \\ A_0 \to iA_0 \\ \gamma^j = i\gamma_j \\ m_0 = -m_0(\cos\lambda + i\gamma_5 \sin\lambda) = -m_0 e^{i\lambda\gamma_5} \end{cases}$$

So the Euclidean spacetime action of system is written as:

$$S_{TI}^E = \int d\tau d^3x \, \bar{\psi}[\gamma_\mu(\partial_\mu - ieA_\mu) + m_0 \cancel{e^{i\lambda\gamma_5}}]\psi$$

~~because of~~:

$$= \int d\tau d^3x \, \bar{\psi}[\gamma_\mu(\partial_\mu - ieA_\mu) - m_0 e^{i\lambda\gamma_5}]\psi$$

$$\cancel{m_0 = -m_0(\cos\lambda + i\gamma_5 \sin\lambda) = -m_0 e^{i\lambda\gamma_5}}$$

Now we apply Fujikawa's method to the action. First, let's consider an infinitesimal chiral transformation defined by:

$$\begin{cases} \psi \to \psi' = e^{\frac{-i\lambda d\phi}{2}\cdot\gamma_5} \cdot \psi \\ \bar{\psi} \to \bar{\psi}' = \cancel{e^{\frac{-i\lambda d\phi}{2}}} \, \bar{\psi} \, e^{\frac{-i\lambda d\phi \gamma_5}{2}} \end{cases}$$

where $\phi \in [0,1]$. Then the partition function Z is transformed as:

$$Z = \int D[\psi, \bar{\psi}] \cdot e^{-S_{TI}^E[\psi, \bar{\psi}]}$$

$$\Rightarrow Z' = \int D[\psi', \bar{\psi}'] \, e^{-S_{TI}'^E[\psi', \bar{\psi}']}$$

let's ~~look~~ see the first term of $S_{TI}^{E'}$:

$$K = \int d\tau d^3x \cdot \bar{\psi} e^{-i\theta\gamma_5} [\gamma_\mu (\partial_\mu - ieA_\mu)] e^{-i\theta\gamma_5} \psi$$

where $\theta = \frac{\pi d\phi}{2}$. Because the anticommutation relation $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$ is satisfied, so:

$$e^{-i\theta\gamma_5} \gamma_\mu = \gamma_\mu e^{i\theta\gamma_5}$$

The Lagrangian of K can be written of:

$$\mathcal{L}_K = \bar{\psi} \gamma_\mu e^{i\theta\gamma_5} (\partial_\mu - ieA_\mu) e^{-i\theta\gamma_5} \psi$$

$$= \bar{\psi} \gamma_\mu (\partial_\mu - ieA_\mu) \psi$$

Next, let's ~~look~~ see the mass term of $S_{TI}^{E'}$:

$$\mathcal{L}_M = -\bar{\psi} e^{-i\theta\gamma_5} m_0 e^{i\pi\gamma_5} e^{-i\theta\gamma_5} \psi$$

$$= -m_0 \bar{\psi} e^{i\pi(1-d\phi)\gamma_5} \psi$$

So the action in Euclidean spacetime is transformed as:

$$S_{TI}^{E'} = \int d\tau d^3x \, \bar{\psi} [\gamma_\mu (\partial_\mu - ieA_\mu) - m_0 e^{i\pi(1-d\phi)\gamma_5}] \psi$$

We should consider the transformation of $D[\psi', \bar{\psi}']$

$$D[\psi', \bar{\psi}'] = J D[\psi, \bar{\psi}']$$

The Jacobian J is written as:

$$\ln J = \cancel{\exp}\, -i \int d\tau d^3x \, d\phi \frac{\lambda e^2}{16\pi^2} \star F^{\mu\nu} F_{\mu\nu}$$

We integrate with respect to the variable ϕ from 0 to 1. ~~d~~
Due to the invariance of the partition function, finally, we arrive at the following expression of S_{TI}^{E}:

$$\cancel{S_{TI}^{E} = \int_0^1 d\phi \cdot \{ \int d\tau d^3x \, \bar{\psi}[\gamma_\mu(\partial_\mu - ieA_\mu) - m_0]\psi - m_0 e^{i\lambda\theta} d\phi}$$

$$S_{TI}^{E} = \int d\tau d^3x \, \bar{\psi}[\gamma_\mu(\partial_\mu - ieA_\mu) - m_0]\psi + i\int d\tau d^3x \frac{\lambda e^2}{16\pi^2} \star F^{\mu\nu} F_{\mu\nu}$$

The first term is the action of a topologycal trivial insulator since the mass $-m_0$ is positive. The second term is the θ term whose θ equal to π in the imaginary time.
Thus, we ~~pro~~ have demonstrated that for 3D topologycal insulators, the θ in θ term is π