

Lecture notes on topological insulators

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I. POINT DEGENERACY BETWEEN ENERGY BANDS

The topology of an energy band is protected by energy gap. Closing of the gap could result in change of topology. We now study the criterion of having a crossing between energy levels in the presence of TRS and SIS. Such an analysis is also related to the study of point degeneracy between energy bands, which is the topic of the next Chap. The discussion here is mainly based on Murakami's analysis of 4-state models (Murakami, 2008a,b).

A. Two-state model - Pauli matrices

Let's start with the two-level case. The Hamiltonian can be expanded by the Pauli matrices,

$$H = d_0(\mathbf{k}) + \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma}. \quad (1.1)$$

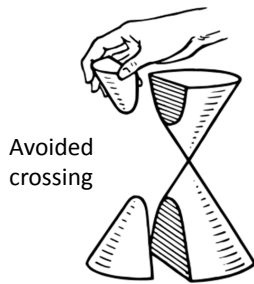


FIG. 1 Two levels could have isolated point degeneracies in 3D parameter space. Therefore, when one varies only one or two parameters, it is likely to miss the target and get an avoided crossing (Fig. is from Wikipedia)

This gives the energy spectrum,

$$\varepsilon_{\pm} = d_0 \pm \sqrt{d_x^2 + d_y^2 + d_z^2}. \quad (1.2)$$

An accidental degeneracy occurs only when $d_x = d_y = d_z = 0$. That is, one needs to tune 3 parameters to have a point degeneracy (see Fig. 1). We say that the degeneracy has **co-dimension 3**. This is first pointed out by von Neumann and Wigner (1929).

As a result, in 2D, it's unlikely to have an accidental degeneracy unless, in addition to (k_x, k_y) , one can vary the third parameter. On the other hand, in a 3D BZ, one can expect to see isolated accidental degenerate points.

The nodal points in graphene cannot be considered as accidental, since they are protected by symmetries. Under time reversal and space inversion ($\Pi = \sigma_x$), we have (ignoring spin)

$$\text{TR} : H^*(\mathbf{k}) = H(-\mathbf{k}), \quad (1.3)$$

$$\text{SI} : \sigma_x H(\mathbf{k}) \sigma_x = H(-\mathbf{k}). \quad (1.4)$$

This leads to

$$(d_x(-\mathbf{k}), d_y(-\mathbf{k}), d_z(-\mathbf{k})) = (d_x(\mathbf{k}), -d_y(\mathbf{k}), d_z(\mathbf{k})), \quad (1.5)$$

$$(d_x(-\mathbf{k}), d_y(-\mathbf{k}), d_z(-\mathbf{k})) = (d_x(\mathbf{k}), -d_y(\mathbf{k}), -d_z(\mathbf{k})) \quad (1.6)$$

With both symmetries, the σ_z term is not allowed. So the co-dimension of the degeneracy reduces to 2, and it's likely to have point degeneracy in a 2D BZ. Furthermore, a small perturbation with only σ_x -term and σ_y -term (respecting both TRS and SIS) could not lift the point degeneracy. For more discussions, see Chap 7 of Bernevig and Hughes, 2013).

On the other hand, if a magnetic field is applied (breaking TRS), or if the sublattices are composed of different atoms (breaking SIS, as in boron nitride), the nodal points are opened.

B. Four-state model - Clifford matrices

Because of the spin degeneracy, a minimal model of a TI usually requires four energy levels, instead of two, and the Hamiltonians are expanded by **Clifford matrices**. Before studying the level crossing, let's first get familiar with the Clifford matrices.

A 4×4 Hamiltonian has 16 real parameters, and can be expanded by 16 bases,

$$\{1, \sigma_x, \sigma_y, \sigma_z\} \otimes \{1, \tau_x, \tau_y, \tau_z\}, \quad (1.7)$$

TABLE I Clifford matrices and their symmetries

Γ	$\Theta\Gamma\Theta^{-1}$	$\Pi\Gamma\Pi^{-1}$
$\Gamma_0 = 1 \otimes 1$	+	+
$\Gamma_1 = \sigma_z \otimes \tau_x$	-	-
$\Gamma_2 = 1 \otimes \tau_y$	-	-
$\Gamma_3 = 1 \otimes \tau_z$	+	+
$\Gamma_4 = \sigma_x \otimes \tau_x$	-	-
$\Gamma_5 = \sigma_y \otimes \tau_x$	-	-
$\Gamma_{12} = \sigma_z \otimes \tau_z$	-	+
$\Gamma_{13} = -\sigma_z \otimes \tau_y$	+	-
$\Gamma_{14} = \sigma_y \otimes 1$	-	+
$\Gamma_{15} = -\sigma_x \otimes 1$	-	+
$\Gamma_{23} = 1 \otimes \tau_x$	+	-
$\Gamma_{24} = -\sigma_x \otimes \tau_z$	-	+
$\Gamma_{25} = -\sigma_y \otimes \tau_z$	-	+
$\Gamma_{34} = -\sigma_x \otimes \tau_y$	+	-
$\Gamma_{35} = \sigma_y \otimes \tau_y$	+	-
$\Gamma_{45} = \sigma_z \otimes 1$	-	+

which are direct products of $\{\text{spin}\} \otimes \{\text{orbital}\}$ (we call these *spin* basis). One can also adopt the basis with $\{\text{orbital}\} \otimes \{\text{spin}\}$ (we call these *orbital* basis). In the former, the components of a state are arranged as $(a_\uparrow, b_\uparrow, a_\downarrow, b_\downarrow)^T$, a and b refer to the probability amplitudes in a -orbital and b -orbital. For the latter, the components are $(a_\uparrow, a_\downarrow, b_\uparrow, b_\downarrow)^T$. Both choices have their advantages and users.

Here we choose the spin basis to define the 16 Clifford matrices in Table I following Bernevig's choice (Chap 11 of [Bernevig and Hughes, 2013](#)). The matrices $\Gamma_1, \dots, \Gamma_5$ are called *generators* of the **Clifford algebra**. They satisfy the anti-commutation relations,

$$\{\Gamma_a, \Gamma_b\} = 2\delta_{ab}, \quad a, b = 1, \dots, 5. \quad (1.8)$$

The next 10 Clifford matrices with two indices are defined as,

$$\Gamma_{ab} = \frac{1}{2i}[\Gamma_a, \Gamma_b]. \quad (1.9)$$

They satisfy (see App. A in [Murakami et al., 2004](#))

$$\{\Gamma_{ab}, \Gamma_{cd}\} = 2\epsilon_{abcde}\Gamma_e + 2\delta_{ac}\delta_{bd} - 2\delta_{ad}\delta_{bc}. \quad (1.10)$$

Also,

$$\{\Gamma_{ab}, \Gamma_c\} = \epsilon_{abcde}\Gamma_{de}. \quad (1.11)$$

In the table we also show the change of sign of a Γ under TR transformation and SI transformation. The TR operator $\Theta = i\sigma_y K \otimes 1$, and the SI operator $\Pi = 1 \otimes \tau_z$, assuming that the conduction band and the valence band have opposite parities (such as s -orbital and p -orbital). If the two bands have the same parity, then the SI operator should be $\Pi = 1 \otimes 1$, and the right-most column in the table would all be +'s.

Notice that the first 6 Clifford matrices, Γ_0 and Γ_a , are even under combined Θ and Π operations,

$$\Theta\Pi\Gamma_a(\Theta\Pi)^{-1} = \Gamma_a. \quad (1.12)$$

Because of the i in the definition of Γ_{ab} shown above, the other 10 Clifford matrices are odd under combined Θ and Π operations,

$$\Theta\Pi\Gamma_{ab}(\Theta\Pi)^{-1} = -\Gamma_{ab}. \quad (1.13)$$

Since $\text{tr}(\mathbf{M} \otimes \mathbf{N}) = \text{tr}\mathbf{M} \text{tr}\mathbf{N}$, we have $\text{tr}\Gamma_a = 0$. In addition, several identities are listed below for later reference:

$$\text{tr}(\Gamma_a\Gamma_b) = 4\delta_{ab}, \quad (1.14)$$

$$\text{tr}(\Gamma_a\Gamma_b\Gamma_c) = 0, \quad (1.15)$$

$$\text{tr}(\Gamma_a\Gamma_b\Gamma_c\Gamma_d) = 4(\delta_{ab}\delta_{cd} + \delta_{ad}\delta_{bc} - \delta_{ac}\delta_{bd}), \quad (1.16)$$

$$\text{tr}(\Gamma_a\Gamma_b\Gamma_c\Gamma_d\Gamma_e) = -4\epsilon_{abcde}, \quad (1.17)$$

$$\Gamma_1\Gamma_2\Gamma_3\Gamma_4\Gamma_5 = -1. \quad (1.18)$$

C. Crossing between four levels

As shown above, the Hamiltonian of a 4-level system can be expanded by 16 Clifford matrices

$$\mathbf{H}(\mathbf{k}) = h_0(\mathbf{k}) + \sum_{a=1}^5 h_a(\mathbf{k})\Gamma_a + \sum_{ab} h_{ab}(\mathbf{k})\Gamma_{ab}, \quad (1.19)$$

where all of the $h(\mathbf{k})$'s are real. If \mathbf{H} has time-reversal symmetry, then according to Table. I, 6 of the $h(\mathbf{k})$'s need to be even, and 10 of the $h(\mathbf{k})$'s odd, functions of \mathbf{k} . They could all exist with proper parities, and the number of Clifford basis cannot be reduced by TRS alone.

1. Inversion symmetry

(a) If conduction band and valence band have the same parity, then the SI operator is

$$\Pi = 1 \otimes 1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (1.20)$$

As a result, all of the signs on the right column of Table I would be "+".

If the system has SIS, then all of the $h(\mathbf{k})$'s need be even functions. If the system has TRS, then 10 of the $h(\mathbf{k})$'s need be odd (see the discussion above). So with both symmetries, only 6 of the Clifford matrices survive,

$$\begin{aligned} \mathbf{H} &= h_0 + h_3\Gamma_3 + h_{13}\Gamma_{13} + h_{23}\Gamma_{23} + h_{34}\Gamma_{34} + h_{35}\Gamma_{35} \\ &= h_0(\mathbf{k}) + \sum_i h_i\Gamma_i, \end{aligned} \quad (1.21)$$

in which i runs over the 5 indices above (3, 13, 23, 34, 35). Also, all of the $h(\mathbf{k})$'s are even functions of \mathbf{k} .

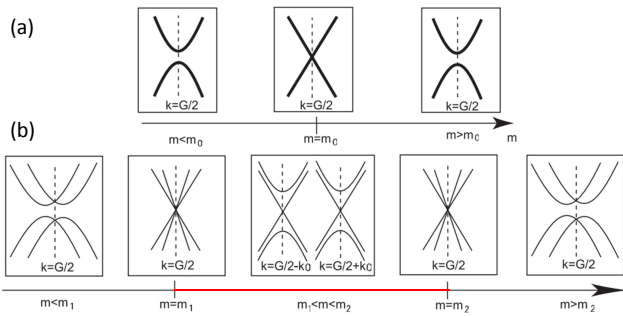


FIG. 2 (a) For a system with both TRS and SIS, if the conduction band and valence band have opposite parities, then one can close the gap at TRIM with one parameter m . (b) If the SIS of the system in (a) is broken, then the critical point m_c could be extended to an interval of gapless region, $m_1 \leq m \leq m_2$. (The figures are from Murakami, 2008a)

Assume the Hamiltonian has energy eigenvalue $\varepsilon(\mathbf{k})$,

$$\mathbf{H}(\mathbf{k})\psi = \varepsilon(\mathbf{k})\psi, \quad (1.22)$$

then

$$\mathbf{H}^2(\mathbf{k})\psi = \varepsilon^2(\mathbf{k})\psi. \quad (1.23)$$

But according to Eqs. (1.10) and (1.11), the anti-commutator of any two of these five Clifford matrices is zero. Therefore,

$$(\mathbf{H} - h_0)^2 = \sum_i h_i^2. \quad (1.24)$$

It follows that,

$$\varepsilon_{\pm}(\mathbf{k}) = h_0(\mathbf{k}) \pm \sqrt{\sum_i h_i^2}. \quad (1.25)$$

The energy levels have global two-fold degeneracy.

To close the energy gap, one needs to tune 5 parameters so that all 5 of the h_i 's are zero. That is, the degenerate point has co-dimension 5. Therefore, varying the 3D momentum \mathbf{k} and an extra parameter m is not enough to close the gap.

(b) On the other hand, if conduction band and valence band have opposite parities, then

$$\mathbf{\Pi} = 1 \otimes \tau_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \quad (1.26)$$

The right column of Table I shows the parities of the Clifford matrices under such a SI operator.

If the system has SIS, then half of the $h(\mathbf{k})$'s need be even, and the other half odd, functions of \mathbf{k} . If the system has TRS, then again 10 of the $h(\mathbf{k})$'s need be odd. So

with both symmetries, only the first 6 Clifford matrices without conflicting $h(\mathbf{k})$ -parities could survive,

$$\mathbf{H} = h_0 + \sum_{a=1}^5 h_a \Gamma_a, \quad (1.27)$$

in which

$$h_a(-\mathbf{k}) = \begin{cases} +h_a(\mathbf{k}), & \text{for } a = 0, 3 \\ -h_a(\mathbf{k}), & \text{for } a = 1, 2, 4, 5 \end{cases} \quad (1.28)$$

According to Eq. (1.8), the anti-commutator of any two of these Γ_a 's is zero. Therefore, with the same argument that leads to Eq. (1.25), we have

$$\varepsilon_{\pm}(\mathbf{k}) = \varepsilon_0(\mathbf{k}) \pm \sqrt{\sum_{a=1}^5 h_a^2}. \quad (1.29)$$

If \mathbf{k} is not a TRIM at $\mathbf{G}/2$, then the co-dimension of the degeneracy is 5. However, if $\mathbf{k} = \mathbf{G}/2$, then $h_{1,2,4,5}(\mathbf{G}/2) = 0$. Therefore, at a TRIM, the co-dimension reduces to 1. That is, one only needs to tune one parameter m to kill h_3 and close the gap at TRIM (see Fig. 2(a)). This analysis applies to 2D as well.

Note: In the analysis above, only TR symmetry and SI symmetry are considered. The codimension can be further reduced if a crystal has additional symmetry, such as mirror symmetry or rotation symmetry. A detailed analysis can be found in Yang and Nagaosa, 2014.

2. Without inversion symmetry

If the system has only TRS, but no SIS, then the energy spectrum does not have global 2-fold degeneracy, only local Kramer degeneracy at TRIM. At some critical parameter, two Kramer pairs might coincide at a TRIM. Away from TRIM, or at the TRIM but away from the critical value, it's unlikely to have the 4-level crossing, and therefore only 2 levels need be considered. As a result, we are back to the 2-level case,

$$\mathbf{H} = d_0(\mathbf{k}) + \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma}. \quad (1.30)$$

The co-dimension is 3. So for a 2D system, there could be isolated point degeneracies in the 3D (\mathbf{k}, m) -space. For a 3D system, there could be isolated point degeneracies in the 3D BZ, and a line of degeneracy in the 4D (\mathbf{k}, m) -space (see Fig. 2(b)).

3. PT symmetry

The discussion above is based on the premise that the system has time-reversal symmetry. When the system also has SIS, then there are only five Clifford matrices (plus Γ_0) in the Hamiltonian, and the spectrum has global two-fold degeneracy. However, it is possible that

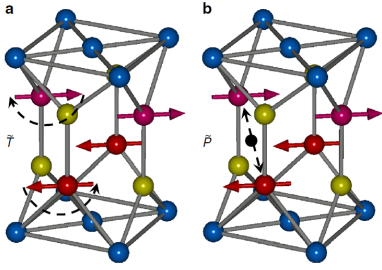


FIG. 3 The spins of the Mn atoms (in red) in CuMnAs have antiferromagnetic order. This configuration is invariant under a combined operation of time reversal (a) and space inversion (b). Fig. from Godinho *et al.*, 2018.

the system has neither TRS, nor SIS, but the combined operation $\Theta\Pi(=\Pi\Theta)$ commutes with H ,

$$\Theta\Pi H(\mathbf{k})(\Theta\Pi)^{-1} = H(\mathbf{k}). \quad (1.31)$$

We say that the system has **PT symmetry** (P for parity). This is possible in antiferromagnetic materials (Tang *et al.*, 2016), as shown in Fig. 3.

If a system has PT symmetry, then an energy eigenstate $\psi_{n\mathbf{k}}$ and its partner $\Theta\Pi\psi_{n\mathbf{k}}$ would have the same energy $\varepsilon_{n\mathbf{k}}$. Furthermore, since $(\Theta\Pi)^2 = -1$, this pair of states are orthogonal to each other. Thus, the energy spectrum has a global two-fold degeneracy.

Furthermore, the Hamiltonian can be expanded by only five Clifford matrices (plus Γ_0). For example, given $\Theta\Pi = i\sigma_y K \otimes \tau_z = -i\Gamma_{25}K$, we can find five matrices in Table I that anti-commute with it and with each other. They can be $\{\Gamma_2, \Gamma_{12}, \Gamma_{23}, \Gamma_{24}, \Gamma_{25}\}$, or $\{\Gamma_5, \Gamma_{15}, \Gamma_{25}, \Gamma_{35}, \Gamma_{45}\}$. Note that they all have "2" or "5" in their indices.

D. Berry curvature near band crossing

1. Two levels

We will use the 2D surface state on a TI as an example. Its effective Hamiltonian near a Dirac point is

$$H_{SS} = \alpha(\boldsymbol{\sigma} \times \mathbf{k})_z + O(k^2), \quad (1.32)$$

The spins in energy eigenstates $\psi_{\pm\mathbf{k}}$ are lying on the x - y plane and perpendicular to \mathbf{k} (opposite directions for the two eigenstates).

When a state with wave vector \mathbf{k} circles around the origin, the direction of its spin also circles once. It is known that when the tip of the spin traces out a loop C , the state acquires a Berry phase $\Gamma_C = \mp\Omega_C/2$, where Ω_C is the solid angle of C with respect to the origin. In the presence case, C is lying on the x - y plane, hence $\Omega_C = 2\pi$ and $\Gamma_C = \mp\pi$.

This is true for any \mathbf{k} -path circling the origin once. Since the Berry phase is an integral of the Berry curva-

ture,

$$\Gamma_C = \int d^2k F_z(\mathbf{k}), \quad (1.33)$$

this implies that the Berry curvature

$$F_z^\pm = \mp\pi\delta^2(\mathbf{k}). \quad (1.34)$$

It's not difficult to see that the Hall conductivity is zero, no matter whether the chemical potential is located below or above the Dirac point (see Fig. 4(a)).

The Dirac point can be opened by magnetic dopants with magnetization m (see Fig. 4(b)),

$$H_{SS} = \alpha(\boldsymbol{\sigma} \times \mathbf{k})_z + m\sigma_z. \quad (1.35)$$

Recall that, if

$$H(\mathbf{k}) = \mathbf{h}(\mathbf{k}) \cdot \boldsymbol{\sigma}, \quad (1.36)$$

then

$$C_1 = \frac{1}{4\pi} \int_{BZ} d^2k \hat{\mathbf{h}} \cdot \frac{\partial \hat{\mathbf{h}}}{\partial k_x} \times \frac{\partial \hat{\mathbf{h}}}{\partial k_y}. \quad (1.37)$$

This is the winding number of the 2D \mathbf{h} -surface over the 2D \mathbf{k} -surface. As a result, the Berry curvature becomes

$$F_z^\pm = \mp \frac{\alpha^2 m}{2(m^2 + \alpha^2 k^2)^{3/2}}. \quad (1.38)$$

If the chemical potential is inside the energy gap, the Hall conductivity is a half-integer,

$$\sigma_H = \frac{e^2}{h} \frac{1}{2\pi} \int d^2k F_z^- = \frac{1}{2} \frac{e^2}{h}. \quad (1.39)$$

Even though the TI has odd number of Dirac point on one surface. The total number of Dirac point for all surfaces should be even. Overall they would contribute an integer Hall conductivity.

For two-level crossing in 3D momentum space, there is a Chern number for a closed surface enclosing the degenerate point. This is called the topological charge of the degenerate point. More details in next chapter.

2. Four levels

In general, for an energy-band n with N -fold degeneracy, its Berry connection is a $N \times N$ matrix,

$$\mathbf{A}_{\alpha\beta}^{(n)}(\boldsymbol{\lambda}) \equiv i \langle n\alpha\boldsymbol{\lambda} | \frac{\partial}{\partial \boldsymbol{\lambda}} | n\beta\boldsymbol{\lambda} \rangle, \quad \alpha, \beta = 1 \cdots N. \quad (1.40)$$

The Berry curvature $F_{k\ell}$ is

$$F_{k\ell} = \partial_k A_\ell - \partial_\ell A_k - i[A_k, A_\ell], \quad k = 1, 2, 3. \quad (1.41)$$

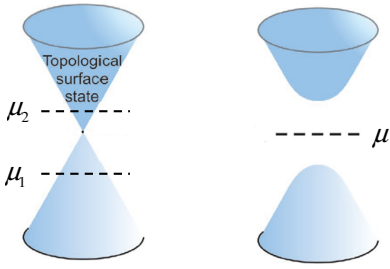


FIG. 4 (a) Dirac cone of the surface state. The chemical potential can be below (μ_1) or above (μ_2) the Dirac point. (b) The Dirac point can be opened by magnetization. Fig. from Liu and Hesjedal, 2021.

For a 2D system, the first Chern number of the band is,

$$C_1 = \frac{1}{2\pi} \int_{BZ} d^2k \operatorname{tr} F_{12}, \quad (1.42)$$

$$\text{where } \operatorname{tr} F_{kl} = \sum_{\alpha=1}^N (F_{\alpha\alpha})_{kl}. \quad (1.43)$$

Taking the trace ensures that the integrand is gauge invariant. For a system with TRS and SIS, $\operatorname{tr} F_{12} = 0$ and the first Chern number vanishes.

For a 4D system (or a 3D system with a tuning parameter), we can introduce the second Chern number,

$$C_2 = \frac{1}{32\pi^2} \int_M d^4x \epsilon_{ijkl} \operatorname{tr} (F_{ij} F_{kl}), \quad (1.44)$$

which is an integral over a closed manifold M . If the dimension of M is less than 4, then $C_2 = 0$. Such a topological invariant appears, for example, in the theory of non-Abelian instanton (M is the 4D Euclidean space-time), or 4D quantum Hall effect (M is the 4D BZ). General formulation of higher Chern numbers, rarely used in condensed matter researches, can be found in Nakahara, 2003.

A formula similar to Eq. (1.37) exists for the second Chern number. Consider a 4-level system with PT symmetry in 4D,

$$H(\mathbf{k}) = \mathbf{h}(\mathbf{k}) \cdot \vec{\Gamma}, \quad (1.45)$$

where Γ_a are 5 Clifford matrices that anti-commute with each other, then

$$C_2 = \frac{3}{8\pi^2} \int_{BZ} d^4k \epsilon_{abcde} \hat{h}_a \partial_1 \hat{h}_b \partial_2 \hat{h}_c \partial_3 \hat{h}_d \partial_4 \hat{h}_e. \quad (1.46)$$

This is the winding number of the 4D \mathbf{h} -surface over the \mathbf{k} -surface (a 4D torus).

For reference, the winding number of a n -sphere over a n -dimensional closed surface M^n is given by

$$w_n = \frac{1}{S_1^n} \int_{M^n} d^n k \epsilon_{za_1 a_2 \dots a_n} \hat{h}_z \partial_1 \hat{h}_{a_1} \partial_2 \hat{h}_{a_2} \dots \partial_n \hat{h}_{a_n}, \quad (1.47)$$

in which

$$S_r^n = \frac{2\pi^{\frac{n+1}{2}}}{\Gamma\left(\frac{n+1}{2}\right)} r^n \quad (1.48)$$

is the surface area of a n -sphere with radius r . Recall that $\Gamma(1) = 1$, $\Gamma(1/2) = \pi^{1/2}$, and $\Gamma(x+1) = x\Gamma(x)$. For example,

$$S_r^2 = 4\pi r^2, \quad S_r^3 = 2\pi^2 r^3, \quad S_r^4 = \frac{8}{3}\pi^2 r^4. \quad (1.49)$$

Exercise

1. (a) With the matrix representation listed in Table I, verify Eq. (1.8).

(b) The matrices Γ_{ab} are defined in Eq. (1.9). Verify that Γ_{1b} , ($b = 2, 3, 4, 5$) are indeed those listed in Table I.

2. In the lecture note, the space inversion operator is either 1 or τ_z , but other forms are possible (Yang and Nagaosa, 2014): First, write

$$\Pi = a_0 + \mathbf{a} \cdot \boldsymbol{\tau}, \quad (1.50)$$

where a_m ($m = 0, 1, 2, 3$) are complex numbers. Two inversions would bring us back to the same state, differing at most by a phase, $\Pi^2 = e^{i\phi}$.

(a) Show that $\Pi = \pm e^{i\phi/2}$, or $\pm e^{i\phi/2} \bar{\mathbf{a}} \cdot \boldsymbol{\tau}$, where $|\bar{\mathbf{a}}|^2 = 1$.

(b) From the following restrictions,

$$[\Theta, \Pi] = 0, \quad (1.51)$$

$$\Pi^\dagger \Pi = 1, \quad (1.52)$$

$$\text{and } (\Theta \Pi)^2 = -1, \quad (1.53)$$

show that (apart from an overall sign)

$$\Pi = \tau_0, \quad \text{or} \quad \cos \theta \tau_z - \sin \theta \tau_x. \quad (1.54)$$

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