

# Lecture notes on topological insulators

Ming-Che Chang

Department of Physics, National Taiwan Normal University, Taipei, Taiwan

(Dated: December 29, 2018)

## Contents

<b>I. More about <math>4 \times 4</math> effective Hamiltonian matrix</b>	1
A. Clifford matrices	1
B. Global two-fold degeneracy	2
C. Berry curvature	2
D. Spin-3/2 representation	3
E. First and Second Chern numbers	4
1. First Chern number	4
2. Second Chern number	5
F. More on the second Chern number	6
1. $C_2$ and projection operator	6
2. $C_2$ and winding number	6
<b>References</b>	7

## I. MORE ABOUT $4 \times 4$ EFFECTIVE HAMILTONIAN MATRIX

Just like the two-state model is very popular in almost every branch of physics, the four-state model is also widely used. In addition to be an effective model of TI, it also appears in, for example, Dirac Hamiltonian, nuclear quadrupole resonance, 4-band Luttinger model, and graphene... etc. Therefore, it's worthy of exploring more about this topic. This chapter can be skipped at first reading, except Sections A and B, if you want to study the chapters on Weyl semimetal.

### A. Clifford matrices

Recall that the Hamiltonian of a two-level system is a  $2 \times 2$  hermitian matrix, which has 4 real parameters. It thus can be expanded by the identity matrix and the three Pauli matrices,

$$H = d_0 1 + d_1 \sigma_x + d_2 \sigma_y + d_3 \sigma_z, \quad (1.1)$$

in which all of the coefficients  $d_i$  are real.

Because of the spin degeneracy, a minimal model of a TI usually requires four energy levels, instead of two. A  $4 \times 4$  Hamiltonian has 16 real parameters, and can be expanded by 16 bases,

$$\{1, \sigma_x, \sigma_y, \sigma_z\} \otimes \{1, \tau_x, \tau_y, \tau_z\}, \quad (1.2)$$

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). Both choices have their advantages and users.

TABLE I Clifford matrices and their symmetries

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

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,

$$\{\Gamma_a, \Gamma_b\} = 2\delta_{ab}, \quad a, b = 1, \dots, 5. \quad (1.3)$$

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

$$\Gamma_{ab} = \frac{1}{2i} [\Gamma_a, \Gamma_b]. \quad (1.4)$$

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

$$\{\Gamma_{ab}, \Gamma_{cd}\} = 2\epsilon_{abcde} \Gamma_e + 2\delta_{ac}\delta_{bd} - 2\delta_{ad}\delta_{bc}. \quad (1.5)$$

Also,

$$\{\Gamma_{ab}, \Gamma_c\} = \epsilon_{abcde} \Gamma_{de}. \quad (1.6)$$

In the table we also show the change of sign of a  $\Gamma$  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  $\Gamma_a$  are even under combined  $\Theta$  and  $\Pi$  operations,

$$\Theta \Pi \Gamma_a (\Theta \Pi)^{-1} = \Gamma_a. \quad (1.7)$$

Because of the  $i$  in the definition of  $\Gamma_{ab}$  shown above, the other 10 Clifford matrices are odd under combined  $\Theta$  and  $\Pi$  operations,

$$\Theta \Pi \Gamma_{ab} (\Theta \Pi)^{-1} = -\Gamma_{ab}. \quad (1.8)$$

Several identities are listed below for later reference:

$$\text{tr}(\Gamma_a \Gamma_b) = \delta_{ab}, \quad (1.9)$$

$$\text{tr}(\Gamma_a \Gamma_b \Gamma_c) = 0, \quad (1.10)$$

$$\text{tr}(\Gamma_a \Gamma_b \Gamma_c \Gamma_d) = 4(\delta_{ab}\delta_{cd} + \delta_{ad}\delta_{bc} - \delta_{ac}\delta_{bd}), \quad (1.11)$$

$$\text{tr}(\Gamma_a \Gamma_b \Gamma_c \Gamma_d \Gamma_e) = -\epsilon_{abcde}, \quad (1.12)$$

$$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 = -1. \quad (1.13)$$

## B. Global two-fold degeneracy

Let's consider the case when a Hamiltonian can be expanded by the first 6 Clifford matrices,

$$\mathbf{H}(\mathbf{k}) = h_0(\mathbf{k}) + \sum_{a=1}^5 h_a(\mathbf{k}) \Gamma_a, \quad (1.14)$$

where  $h_a(\mathbf{k})$  are real functions. If this system has TRS, such that  $\Theta \mathbf{H}(\mathbf{k}) \Theta^{-1} = \mathbf{H}(-\mathbf{k})$ , then

$$h_a(-\mathbf{k}) = \begin{cases} +h_a(\mathbf{k}), & \text{for } a = 0, 3 \\ -h_a(\mathbf{k}), & \text{for } a = 1, 2, 4, 5 \end{cases} \quad (1.15)$$

This automatically implies SIS,  $\Pi \mathbf{H}(\mathbf{k}) \Pi^{-1} = \mathbf{H}(-\mathbf{k})$ . With both TRS and SIS, the energy spectrum would have global two-fold degeneracy.

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

$$\mathbf{H}(\mathbf{k})\psi = \varepsilon(\mathbf{k})\psi, \quad (1.16)$$

then

$$\mathbf{H}^2(\mathbf{k})\psi = \varepsilon^2(\mathbf{k})\psi. \quad (1.17)$$

But from Eq. (1.3), we get

$$(\mathbf{H} - h_0)^2 = \sum_{a=1}^5 h_a^2. \quad (1.18)$$

Therefore,

$$\varepsilon_{\pm}(\mathbf{k}) = h_0(\mathbf{k}) \pm \sqrt{\sum_{a=1}^5 h_a^2}. \quad (1.19)$$

Thus, indeed the energy levels have global two-fold degeneracy.

## C. Berry curvature

We now calculate the Berry curvature of this  $4 \times 4$  Hamiltonian. The  $h_0$  term can be dropped since it does not affect the Berry curvature. To facilitate the calculation, it helps to introduce the projection operator. First write

$$\mathbf{H} = \sum_{a=1}^5 h_a(\mathbf{k}) \Gamma_a = h \tilde{\mathbf{H}}, \quad (1.20)$$

where

$$\tilde{\mathbf{H}} = \hat{\mathbf{h}} \cdot \vec{\Gamma}, \quad (1.21)$$

and  $\hat{\mathbf{h}}$  is the unit vector of the 5-dimensional vector  $\mathbf{h}$ . If  $|\pm\rangle$  are the energy eigenstates (each spans a 2D Hilbert space) with energies  $\varepsilon_{\pm}$ , then

$$\tilde{\mathbf{H}}^2 = |\hat{\mathbf{h}}|^2 = 1, \quad (1.22)$$

$$\tilde{\mathbf{H}}|+\rangle = +|+\rangle, \quad (1.23)$$

$$\tilde{\mathbf{H}}|-\rangle = -|-\rangle. \quad (1.24)$$

The projection operators that pick up the  $|\pm\rangle$  states can be written as,

$$P_{\pm} = \frac{1}{2} (1 \pm \tilde{\mathbf{H}}) = \frac{1}{2} (1 \pm \hat{\mathbf{h}} \cdot \vec{\Gamma}). \quad (1.25)$$

It satisfies

$$P_{\pm}^2 = P_{\pm}, \quad P_+ P_- = P_- P_+ = 0, \quad (1.26)$$

and

$$\mathbf{H} = h (P_+ - P_-) = \varepsilon_+ P_+ + \varepsilon_- P_-. \quad (1.27)$$

Recall that the non-Abelian Berry curvature is (see ??)

$$\mathbf{F}_{k\ell} = \partial_k \mathbf{A}_{\ell} - \partial_{\ell} \mathbf{A}_k - i[\mathbf{A}_k, \mathbf{A}_{\ell}], \quad (1.28)$$

where

$$(\mathbf{A}_{\ell})_{\alpha\beta} = i \langle \alpha | \frac{\partial}{\partial k_{\ell}} | \beta \rangle, \quad (1.29)$$

in which  $k, \ell = 1, 2, 3$  are space indices, and  $\alpha, \beta = 1, 2, 3, 4$  are energy-level indices. It can also be written as

$$\begin{aligned} (F_{k\ell})_{\alpha\beta} &= i (\langle \partial_k \alpha | \partial_{\ell} \beta \rangle - \langle \partial_{\ell} \alpha | \partial_k \beta \rangle) \\ &\quad - i \sum_{\gamma=1}^4 (\langle \partial_k \alpha | \gamma \rangle \langle \gamma | \partial_{\ell} \beta \rangle - \langle \partial_{\ell} \alpha | \gamma \rangle \langle \gamma | \partial_k \beta \rangle). \end{aligned} \quad (1.30)$$

One can insert a complete set to the first line  $\sum_{\gamma=1}^4 |\gamma\rangle \langle \gamma| = 1$ , then the two lines are the same and cancel with each other. That is, the Berry curvature in the whole Hilbert space (which is model-dependent, of course) is always zero. It is non-zero only in a subspace.

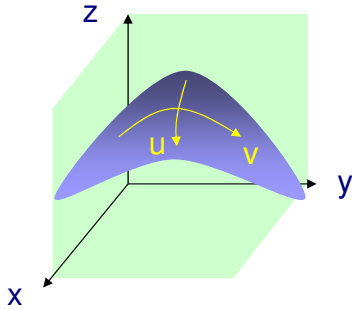


FIG. 1 A subspace of an Euclidean space can be curved.

An analogy of this is that the 3D Euclidean space we live in is flat, but a 2D surface in it can be curved (Fig. 1).

For example, consider the nuclear quadrupole resonance in ???. The Hilbert space there has four dimensions. If one calculates its Berry curvature, the result would be zero. Only after the projections to subspaces ( $|m\rangle = 3/2, |m\rangle = 1/2$ ) can we get non-zero Berry curvatures  $F_{\theta\phi}^{3/2}, F_{\theta\phi}^{1/2}$ .

To get the Berry curvature  $F_{k\ell}^{\pm}$  for a subspace ( $|+\rangle$  or  $|-\rangle$ ), one restricts  $\alpha, \beta, \gamma$  to (1,2) for  $|-\rangle$ ; or (3,4) for  $|+\rangle$ . Other than that, the equation above remains the same, Again one can insert a complete set to the first line  $\sum_{\gamma=1}^4 |\gamma\rangle\langle\gamma| = 1$ , but now there is an incomplete cancellation between the two lines, and

$$(F_{k\ell})_{\alpha\beta}^{\pm} = i \sum_{\bar{\gamma} \in \text{out}} (\langle \partial_k \alpha | \bar{\gamma} \rangle \langle \bar{\gamma} | \partial_\ell \beta \rangle - \langle \partial_\ell \alpha | \bar{\gamma} \rangle \langle \bar{\gamma} | \partial_k \beta \rangle), \quad (1.31)$$

in which  $\bar{\gamma}$  runs over states *outside* of the subspace that we are interested in.

It follows from Eq. (1.31) that the Berry curvature can also be expressed in projection operators  $P_{\pm} = \sum_{\alpha \in \pm} |\alpha\rangle\langle\alpha|$ ,

$$\hat{F}_{k\ell}^{\pm} \equiv \sum_{\alpha\beta \in \pm} |\alpha\rangle (F_{k\ell})_{\alpha\beta}^{\pm} \langle\beta| \quad (1.32)$$

$$= i \left[ \frac{\partial P_{\pm}}{\partial k_k} P_{\mp} \frac{\partial P_{\pm}}{\partial k_\ell} - (k \leftrightarrow \ell) \right]. \quad (1.33)$$

One can rewrite  $P_{\mp} = 1 - P_{\pm}$ , use  $(\partial_k P_{\pm}) P_{\pm} = -P_{\pm} \partial_k P_{\pm}$ , and write the Berry curvature in an alternative form,

$$\hat{F}_{k\ell}^{\pm} = iP_{\pm} \left[ \frac{\partial P_{\pm}}{\partial k_k}, \frac{\partial P_{\pm}}{\partial k_\ell} \right]. \quad (1.34)$$

A closely related Berry curvature is

$$\hat{F}_{ab}^{\pm} = iP_{\pm} \left[ \frac{\partial P_{\pm}}{\partial h_a}, \frac{\partial P_{\pm}}{\partial h_b} \right], \quad (1.35)$$

where  $a, b = 1, 2, \dots, 5$  are the Clifford indices. The two Berry curvatures defined on different domains in

Eq. (1.34) and (1.35) can be related by a pull-back transformation,

$$\hat{F}_{k\ell}^{\pm} = \sum_{ab} \hat{F}_{ab}^{\pm} \frac{\partial h_a}{\partial k_k} \frac{\partial h_b}{\partial k_\ell}. \quad (1.36)$$

For more discussion, see Murakami *et al.*, 2004.

#### D. Spin-3/2 representation

The spin matrices for a spin-3/2 particle are (see ??)

$$J_1 = \begin{pmatrix} 0 & \sqrt{3}/2 & 0 & 0 \\ \sqrt{3}/2 & 0 & 1 & 0 \\ 0 & 1 & 0 & \sqrt{3}/2 \\ 0 & 0 & \sqrt{3}/2 & 0 \end{pmatrix}, \quad (1.37)$$

$$J_2 = \begin{pmatrix} 0 & -i\sqrt{3}/2 & 0 & 0 \\ i\sqrt{3}/2 & 0 & -i & 0 \\ 0 & i & 0 & -i\sqrt{3}/2 \\ 0 & 0 & i\sqrt{3}/2 & 0 \end{pmatrix}, \quad (1.38)$$

$$J_3 = \begin{pmatrix} 3/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & -3/2 \end{pmatrix}. \quad (1.39)$$

A  $4 \times 4$  matrix can be expanded using either the Clifford matrices or the spin matrices (Avron *et al.*, 1988),

$$H = \sum_{a=1}^5 h_a \Gamma_a + \sum_{ab} h_{ab} \Gamma_{ab} \quad (1.40)$$

$$= \sum_{\mu\nu=0}^3 A_{\mu\nu} J_{\mu} J_{\nu}, \quad J_0 = 1. \quad (1.41)$$

If there is TRS, then the Hamiltonian is

$$H(Q) = \sum_{k\ell=1}^3 Q_{k\ell} J_k J_\ell, \quad (1.42)$$

where  $Q_{k\ell}$  is a  $3 \times 3$ , real, symmetric, traceless matrix with 5 independent parameters.

The quadrupole tensor  $Q$  itself can be considered as a vector in a 5D space. For example, choose the following basis,

$$Q_1 = \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, Q_2 = \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad (1.43)$$

$$Q_3 = \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, Q_4 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (1.44)$$

$$Q_5 = \frac{1}{3} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}. \quad (1.45)$$

Their inner products can be defined as,

$$(\mathbf{Q}_a, \mathbf{Q}_b) = \frac{3}{2} \text{tr}(\mathbf{Q}_a \mathbf{Q}_b) = \delta_{ab}. \quad (1.46)$$

Expand  $\mathbf{Q}$  as,

$$\mathbf{Q} = \sum_a \tilde{h}_a \mathbf{Q}_a, \quad (1.47)$$

then the inner product between two “vectors”  $\mathbf{Q}$  and  $\mathbf{Q}'$  are,

$$(\mathbf{Q}, \mathbf{Q}') = \frac{3}{2} \text{tr}(\mathbf{Q} \mathbf{Q}'), \quad (1.48)$$

and

$$|\mathbf{Q}|^2 = \sum_a \tilde{h}_a^2. \quad (1.49)$$

Consider the following matrices,

$$\tilde{\Gamma}_1 = \mathbf{H}(\mathbf{Q}_1) = \frac{1}{\sqrt{3}} (J_2 J_3 + J_3 J_2) = \sigma_3 \otimes \sigma_2, \quad (1.50)$$

$$\tilde{\Gamma}_2 = \mathbf{H}(\mathbf{Q}_2) = \frac{1}{\sqrt{3}} (J_3 J_1 + J_1 J_3) = \sigma_3 \otimes \sigma_1, \quad (1.51)$$

$$\tilde{\Gamma}_3 = \mathbf{H}(\mathbf{Q}_3) = \frac{1}{\sqrt{3}} (J_1 J_2 + J_2 J_1) = \sigma_2 \otimes 1, \quad (1.52)$$

$$\tilde{\Gamma}_4 = \mathbf{H}(\mathbf{Q}_4) = \frac{1}{\sqrt{3}} (J_1^2 - J_2^2) = \sigma_1 \otimes 1, \quad (1.53)$$

$$\tilde{\Gamma}_5 = \mathbf{H}(\mathbf{Q}_5) = \frac{1}{3} (2J_3^2 - J_1^2 - J_2^2) = \sigma_3 \otimes \sigma_3. \quad (1.54)$$

Apart from signs, they are  $\Gamma_{13}, \Gamma_1, \Gamma_{14}, \Gamma_{15}, \Gamma_{12}$  in Table I. According to Eqs. (1.5) and (1.6), these  $\tilde{\Gamma}_a$ 's can also be generators of the Clifford algebra. That is,

$$\{\tilde{\Gamma}_a, \tilde{\Gamma}_b\} = 2\delta_{ab}, \quad a, b = 1, \dots, 5. \quad (1.55)$$

The Hamiltonian can be regarded as a linear operator acting on the vector  $\mathbf{Q}$ . Given  $\mathbf{Q} = \sum \tilde{h}_a \mathbf{Q}_a$ , one has

$$\mathbf{H}(\mathbf{Q}) = \sum_a \tilde{h}_a \mathbf{H}(\mathbf{Q}_a) \quad (1.56)$$

$$= \sum_a \tilde{h}_a \tilde{\Gamma}_a. \quad (1.57)$$

This is analogous to Eq. (1.14), but with a different Clifford basis. Also,

$$[\mathbf{H}(\mathbf{Q})]^2 = |\tilde{\mathbf{h}}|^2 = |\mathbf{Q}|^2. \quad (1.58)$$

The eigenvalues of  $\mathbf{H}(\mathbf{Q})$  are  $\pm |\tilde{\mathbf{h}}|$ , as shown earlier.

A rotation in the 5D  $\mathbf{Q}$ -space is an **isometric transformation** that preserves distance, and vice versa. That is, if  $|\tilde{\mathbf{h}}'| = |\tilde{\mathbf{h}}|$ , then  $\mathbf{Q}'$  and  $\mathbf{Q}$  are related by a  $\text{SO}(5)$  rotation. Furthermore, since  $\mathbf{H}(\mathbf{Q}')$  and  $\mathbf{H}(\mathbf{Q})$  have the same eigenvalues, they are linked by a unitary transformation that corresponds to a rotation,

$$\mathbf{H}(\mathbf{Q}') = \mathbf{U} \mathbf{H}(\mathbf{Q}) \mathbf{U}^{-1}. \quad (1.59)$$

Note that a general spin- $j$  model has  $\text{SO}(3)$  symmetry, but only the *spin-3/2 system with TRS* can have this extra  $\text{SO}(5)$  symmetry.(?) For more discussions, see [Avron et al., 1989](#).

## E. First and Second Chern numbers

### 1. First Chern number

For a system with  $N$  energy levels, the Berry curvature  $F_{k\ell}$  is a  $N \times N$  matrix. Given an insulator with  $N$  filled levels and  $M$  empty levels, only the filled levels contribute to the electronic topological phase. For a 2D system, the first Chern number is,

$$C_1 = \frac{1}{2\pi} \int_{BZ} d^2k \text{tr} F_{12}, \quad (1.60)$$

$$\text{tr} F_{k\ell} = \sum_{\alpha=1}^N (F_{\alpha\alpha})_{k\ell}. \quad (1.61)$$

If a level  $\alpha$  is gapped from the rest of the filled levels, then its first Chern number is well-defined,

$$C_1^\alpha = \frac{1}{2\pi} \int_{BZ} d^2k (F_{\alpha\alpha})_{12}. \quad (1.62)$$

However, if it tangles with other levels, then  $C_1^\alpha$  is not gauge invariant (from the multi-level perspective) and may not be an integer due to level crossing ([Soluyanov and Vanderbilt, 2012](#)).

The Hamiltonian can be written as a sum of two parts,

$$H = \sum_{\alpha=1}^N \varepsilon_\alpha(\mathbf{k}) |\alpha\mathbf{k}\rangle \langle \alpha\mathbf{k}| + \sum_{\alpha=N+1}^{N+M} \varepsilon_\alpha(\mathbf{k}) |\alpha\mathbf{k}\rangle \langle \alpha\mathbf{k}|. \quad (1.63)$$

If we are only interested in its topology, then it is alright to merge and deform the energy levels, so that all of the filled levels have the same energy  $\varepsilon_-$ , and all of the empty levels have the energy  $\varepsilon_+$ . The topology is not changed as long as the insulating gap is not closed. After the simplification,

$$\begin{aligned} H &= \varepsilon_- \sum_{\alpha=1}^N |\alpha\mathbf{k}\rangle \langle \alpha\mathbf{k}| + \varepsilon_+ \sum_{\alpha=N+1}^{N+M} |\alpha\mathbf{k}\rangle \langle \alpha\mathbf{k}| \\ &= \varepsilon_- P_- + \varepsilon_+ P_+, \end{aligned} \quad (1.64)$$

where

$$P_- = \sum_{\alpha=1}^N |\alpha\mathbf{k}\rangle \langle \alpha\mathbf{k}|, \quad P_+ = \sum_{\alpha=N+1}^{N+M} |\alpha\mathbf{k}\rangle \langle \alpha\mathbf{k}|. \quad (1.66)$$

They project a state to the subspaces of empty levels or filled levels. This is a generalization of the projection operators in I.C.

The Berry curvature of each subspace can be written as (see Eq. (1.34))

$$\hat{F}_{k\ell}^\pm = iP_\pm \left[ \frac{\partial P_\pm}{\partial k_k}, \frac{\partial P_\pm}{\partial k_\ell} \right]. \quad (1.67)$$

Also, the Chern number in Eq. (1.60) can be written as

$$C_1 = \frac{i}{2\pi} \int_{BZ} d^2k \text{tr} \left( P_- \left[ \frac{\partial P_-}{\partial k_1}, \frac{\partial P_-}{\partial k_2} \right] \right). \quad (1.68)$$

For example, if

$$\mathbf{H}(\mathbf{k}) = \mathbf{h}(\mathbf{k}) \cdot \boldsymbol{\sigma}, \quad (1.69)$$

then one can show that,

$$C_1 = \frac{1}{4\pi} \int_{BZ} d^2k \hat{\mathbf{h}} \cdot \frac{\partial \hat{\mathbf{h}}}{\partial k_x} \times \frac{\partial \hat{\mathbf{h}}}{\partial k_y}. \quad (1.70)$$

This is the winding number of the 2D  $\mathbf{h}$ -surface over the 2D  $\mathbf{k}$ -surface.

## 2. Second Chern number

The second Chern number is defined as (see App. ??)

$$C_2 = \frac{1}{32\pi^2} \int_M d^4x \epsilon_{ijkl} \text{tr}(\mathbf{F}_{ij}\mathbf{F}_{kl}), \quad (1.71)$$

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, see below), or 4D quantum Hall effect ( $M$  is the 4D BZ, see next chapter). General formulation of higher Chern numbers, rarely used in condensed matter researches, can be found in App. ??.

### ■ Instanton

In the following, we cite the instanton in SU(2) gauge field theory as an example to illustrate that  $C_2$  is a topological invariant. An instanton is a classical soliton of Yang-Mills field in *Euclidean* space-time (see Chap 6 of [Coleman, 1985](#)). Its *topological charge* (aka **Pontrygain index**) is given by the second Chern number,

$$Q_T = \frac{1}{8\pi^2} \int_M d^4x \frac{1}{4} \epsilon_{ijkl} \text{tr}(\mathbf{F}_{ij}\mathbf{F}_{kl}). \quad (1.72)$$

At first, let's introduce the **Chern-Simons identity**:

$$\frac{1}{4} \epsilon_{ijkl} \text{tr}(\mathbf{F}_{ij}\mathbf{F}_{kl}) = \partial_i \left[ \epsilon_{ijkl} \text{tr} \left( \mathbf{A}_j \partial_k \mathbf{A}_l - \frac{2i}{3} \mathbf{A}_j \mathbf{A}_k \mathbf{A}_l \right) \right]. \quad (1.73)$$

Be aware that the same symbol  $i$  is used for both a subscript and an imaginary number ( $i, j, k, l = 1, \dots, 4$ ).

*Pf:* First,

$$\mathbf{F}_{kl} = \partial_k \mathbf{A}_l - i \mathbf{A}_k \mathbf{A}_l - (k \leftrightarrow l), \quad (1.74)$$

so

$$\begin{aligned} \text{LHS} &= \epsilon_{ijkl} \text{tr}(\partial_i \mathbf{A}_j - i \mathbf{A}_i \mathbf{A}_j)(\partial_k \mathbf{A}_l - i \mathbf{A}_k \mathbf{A}_l) \\ &= \epsilon_{ijkl} \text{tr}(\partial_i \mathbf{A}_j \partial_k \mathbf{A}_l - 2i \mathbf{A}_i \mathbf{A}_j \partial_k \mathbf{A}_l). \end{aligned} \quad (1.75)$$

The quartic term is zero because  $\epsilon_{ijkl} = -\epsilon_{lij k}$ , while the trace has cyclic symmetry. Next, use

$$\epsilon_{ijkl} \text{tr}(\partial_i \mathbf{A}_j \partial_k \mathbf{A}_l) = \epsilon_{ijkl} \partial_k \text{tr}(\partial_i \mathbf{A}_j \mathbf{A}_l), \quad (1.76)$$

$$\epsilon_{ijkl} \text{tr}(\mathbf{A}_i \mathbf{A}_j \partial_k \mathbf{A}_l) = \frac{1}{3} \epsilon_{ijkl} \partial_k \text{tr}(\mathbf{A}_i \mathbf{A}_j \mathbf{A}_l). \quad (1.77)$$

It follows that,

$$\text{LHS} = \epsilon_{ijkl} \partial_k \text{tr} \left( \partial_i \mathbf{A}_j \mathbf{A}_l - \frac{2i}{3} \mathbf{A}_i \mathbf{A}_j \mathbf{A}_l \right) \quad (1.78)$$

$$= \partial_i \left[ \epsilon_{ijkl} \text{tr} \left( \mathbf{A}_j \partial_k \mathbf{A}_l - \frac{2i}{3} \mathbf{A}_j \mathbf{A}_k \mathbf{A}_l \right) \right]. \quad (1.79)$$

End of proof.

Note: If  $(\mathbf{A}_\ell)_{\alpha\beta} \equiv -i \langle \alpha | \frac{\partial}{\partial k_\ell} | \beta \rangle$ , then the coefficient of the second term would be  $+2i/3$ , instead of  $-2i/3$ .

The CS identity shows that the LHS (aka *topological charge density*) can be written as a total derivative  $\partial_i J_i$ . At infinity, the field strength  $\mathbf{F}_{kl} \rightarrow 0$ , so the gauge potential is a pure gauge,

$$\mathbf{A}_k \rightarrow i \mathbf{U}^\dagger \partial_k \mathbf{U}. \quad (1.80)$$

The *topological current density* can be written as,

$$J_i \equiv \epsilon_{ijkl} \text{tr} \left( \mathbf{A}_j \partial_k \mathbf{A}_l - \frac{2i}{3} \mathbf{A}_j \mathbf{A}_k \mathbf{A}_l \right) \quad (1.81)$$

$$= \epsilon_{ijkl} \text{tr} \left( \frac{1}{2} \mathbf{A}_j \mathbf{F}_{kl} + \frac{i}{3} \mathbf{A}_j \mathbf{A}_k \mathbf{A}_l \right) \quad (1.82)$$

$$= \frac{1}{3} \epsilon_{ijkl} \text{tr}(\mathbf{U}^\dagger \partial_j \mathbf{U} \mathbf{U}^\dagger \partial_k \mathbf{U} \mathbf{U}^\dagger \partial_l \mathbf{U}). \quad (1.83)$$

Thus,

$$C_2 = \frac{1}{8\pi^2} \int_M d^4x \partial_i J_i = \frac{1}{8\pi^2} \int_{S_\infty^3} dS_i J_i, \quad (1.84)$$

where  $S_\infty^3$  is a 3D sphere at infinity in the 4D Euclidean space.

We now show that the integral above is an integer:  $U(x)$  defines a mapping from an unit sphere  $x \in S_1^3$  to  $U(x) \in \text{SU}(2)$ , which is also a 3-sphere. One can parametrize  $x \in S_1^3$  by  $\psi_1, \psi_2, \psi_3$  ([Dittrich and Reuter, 1986](#)),

$$x_1 = \sin \psi_1 \sin \psi_2 \sin \psi_3, \quad (1.85)$$

$$x_2 = \sin \psi_1 \sin \psi_2 \cos \psi_3, \quad (1.86)$$

$$x_3 = \sin \psi_1 \cos \psi_2, \quad (1.87)$$

$$x_4 = \cos \psi_1. \quad (1.88)$$

The SU(2) sphere is parametrized by the Euler angles  $\theta_1, \theta_2, \theta_3$ ,

$$\mathbf{U}(x) = e^{\frac{i}{2} \theta_1 \sigma_3} e^{\frac{i}{2} \theta_2 \sigma_2} e^{\frac{i}{2} \theta_3 \sigma_3}, \quad (1.89)$$

in which  $\theta_1 \in [0, 2\pi]$ ,  $\theta_2 \in [0, \pi]$ , and  $\theta_3 \in [0, 4\pi]$  ([Gottfried, 1989](#)). Note that for SO(3),  $\theta_3$  is restricted  $[0, 2\pi]$ .

Use

$$\frac{\partial \mathbf{U}}{\partial x_i} = \frac{\partial \mathbf{U}}{\partial \theta_a} \frac{\partial \theta_a}{\partial x_i}, \quad (1.90)$$

then

$$\begin{aligned} J_i &= \frac{1}{3} \epsilon_{ijkl} \partial_j \theta_a \partial_k \theta_b \partial_l \theta_c \text{tr}(\mathbf{U}^\dagger \partial_a \mathbf{U} \mathbf{U}^\dagger \partial_b \mathbf{U} \mathbf{U}^\dagger \partial_c \mathbf{U}) \\ &= 3! \frac{1}{3} \epsilon_{ijkl} \partial_j \theta_1 \partial_k \theta_2 \partial_l \theta_3 \text{tr}(\mathbf{U}^\dagger \partial_1 \mathbf{U} \mathbf{U}^\dagger \partial_2 \mathbf{U} \mathbf{U}^\dagger \partial_3 \mathbf{U}). \end{aligned} \quad (1.91)$$

The surface element

$$\epsilon_{ijkl} \partial_j \theta_1 \partial_k \theta_2 \partial_l \theta_3 dS_i = d\theta_1 d\theta_2 d\theta_3. \quad (1.92)$$

Therefore,

$$C_2 = \frac{1}{4\pi^2} \int d\theta_1 d\theta_2 d\theta_3 \operatorname{tr} (U^\dagger \partial_1 U U^\dagger \partial_2 U U^\dagger \partial_3 U). \quad (1.93)$$

It is left as an exercise to show that

$$\operatorname{tr} (U^\dagger \partial_1 U U^\dagger \partial_2 U U^\dagger \partial_3 U) = \frac{1}{4} \sin \theta_2. \quad (1.94)$$

Therefore,

$$\begin{aligned} C_2 &= \frac{n}{16\pi^2} \int_0^{2\pi} d\theta_1 \int_0^\pi d\theta_2 \int_0^{4\pi} d\theta_3 \sin \theta_2 \\ &= n \in Z, \end{aligned} \quad (1.95)$$

where  $n$  is the winding number of the mapping  $S_1^3 \rightarrow \text{SU}(2)$ .

In general, there is higher Chern number  $C_n$  in  $2n$ -dimension. We then could have the following integral (Ryu *et al.*, 2010),

$$\begin{aligned} &\nu_{2n-1} \\ &= N_{2n-1} \int_M d^{2n-1}x \epsilon_{i_1 \dots i_{2n-1}} \operatorname{tr} (U^\dagger \partial_{i_1} U \dots U^\dagger \partial_{i_{2n-1}} U), \end{aligned} \quad (1.96)$$

where  $M$  is a closed  $(2n - 1)$ -dimensional manifold, and  $U$  is a  $U(N)$  matrix. With proper normalization, this is an integer under continuous deformation of  $M$ .

Note: Similar integral with even number of  $U^\dagger dU$  is always zero. This is a result of the cyclic symmetry of the trace, plus the fact that  $\epsilon_{i_1 i_2 \dots i_{2n}} = -\epsilon_{i_{2n} i_1 \dots i_{2n-1}}$ .

## F. More on the second Chern number

### 1. $C_2$ and projection operator

Similar to  $C_1$ ,  $C_2$  can also be written in projection operators (Chap 13 of Bernevig and Hughes, 2013),

$$C_2 = \frac{1}{8\pi^2} \int_{BZ} d^4k \epsilon_{ijkl} \operatorname{tr} \left( P_+ \frac{\partial P_-}{\partial k_i} \frac{\partial P_-}{\partial k_j} P_+ \frac{\partial P_-}{\partial k_k} \frac{\partial P_-}{\partial k_l} \right), \quad (1.97)$$

where  $P_\pm$  are defined in Eq. (1.66), and one needs to trace over filled levels below the chemical potential.

*Pf.* First, use

$$\hat{F}_{k\ell}^\pm = i \left[ \frac{\partial P_\pm}{\partial k_k} P_\mp \frac{\partial P_\pm}{\partial k_\ell} - (k \leftrightarrow \ell) \right]. \quad (1.98)$$

Then

$$\frac{1}{4} \epsilon_{ijkl} \operatorname{tr} (F_{ij}^- F_{kl}^-) = -\frac{1}{4} \epsilon_{ijkl} \operatorname{tr} \left\{ \left[ \frac{\partial P_-}{\partial k_i} P_+ \frac{\partial P_-}{\partial k_j} - (i \leftrightarrow j) \right] \left[ \frac{\partial P_-}{\partial k_k} P_+ \frac{\partial P_-}{\partial k_l} - (k \leftrightarrow l) \right] \right\} \quad (1.99)$$

$$\begin{aligned} &= -\frac{1}{4} \epsilon_{ijkl} \operatorname{tr} \left( \frac{\partial P_-}{\partial k_i} P_+ \frac{\partial P_-}{\partial k_j} \frac{\partial P_-}{\partial k_k} P_+ \frac{\partial P_-}{\partial k_l} - \frac{\partial P_-}{\partial k_i} P_+ \frac{\partial P_-}{\partial k_j} \frac{\partial P_-}{\partial k_l} P_+ \frac{\partial P_-}{\partial k_k} \right. \\ &\quad \left. - \frac{\partial P_-}{\partial k_j} P_+ \frac{\partial P_-}{\partial k_i} \frac{\partial P_-}{\partial k_k} P_+ \frac{\partial P_-}{\partial k_l} + \frac{\partial P_-}{\partial k_j} P_+ \frac{\partial P_-}{\partial k_i} \frac{\partial P_-}{\partial k_l} P_+ \frac{\partial P_-}{\partial k_k} \right) \end{aligned} \quad (1.100)$$

$$= \epsilon_{ijkl} \operatorname{tr} \left( P_+ \frac{\partial P_-}{\partial k_i} \frac{\partial P_-}{\partial k_j} P_+ \frac{\partial P_-}{\partial k_k} \frac{\partial P_-}{\partial k_l} \right). \quad (1.101)$$

In the last equation, we have used the cyclic invariance of the trace to move the projection operators to the right positions. The  $C_2$  in Eq. (1.97) then follows.

### 2. $C_2$ and winding number

A formula similar to Eq. (1.70) exists in  $4$ -level system with  $TRS$ . That is, if

$$H(\mathbf{k}) = \mathbf{h}(\mathbf{k}) \cdot \vec{\Gamma}, \quad (1.102)$$

where  $\Gamma_a$  are the 5 generators of the Clifford algebra, then

$$C_2 = \frac{3}{8\pi^2} \int_{BZ} d^4k \epsilon_{abcde} \hat{h}_a \partial_1 \hat{h}_b \partial_2 \hat{h}_c \partial_3 \hat{h}_d \partial_4 \hat{h}_e. \quad (1.103)$$

This is the winding number of the 4D  $\mathbf{h}$ -surface over the 4D  $\mathbf{k}$ -surface. The readers are invited to prove this using Eq. (1.101).

In general, the winding number of a  $n$ -sphere over a  $n$ -dimensional closed surface  $M^n$  is given by

$$w_n = \frac{1}{S_1^n} \int_{M^n} d^n k \epsilon_{z a_1 a_2 \dots a_n} \hat{h}_z \partial_1 \hat{h}_{a_1} \partial_2 \hat{h}_{a_2} \dots \partial_n \hat{h}_{a_n}, \quad (1.104)$$

in which

$$S_r^n = \frac{2\pi^{\frac{n+1}{2}}}{\Gamma(\frac{n+1}{2})} r^n \quad (1.105)$$

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,

$$S_r^2 = 4\pi r^2, \quad S_r^3 = 2\pi^2 r^3, \quad S_r^4 = \frac{8}{3}\pi^2 r^4. \quad (1.106)$$

Example related to the mapping  $T^3 \rightarrow S^3$  can be found in Eq. (??) of previous chapter.

The formulation here does not apply to the TI directly. For a 3D TI, the base space (BZ) is 3D, instead of 4D, and the second Chern number is irrelevant. For a 2D TI, the base space is 2D ( $T^2$ ). Even though its  $C_1$  can be calculated, but the result is zero due to the TRS. The topology is hidden in the  $Z_2$  topological number.

As we have mentioned,  $C_2$  is relevant in a 4D QH system (which has TRS, unlike the 2D QH system). It is found by Qi and Zhang that the 3D TI can be inferred from the 4D QHE by dimensional reduction. This is the subject of next chapter.

### Exercise

1. If the SI operator is  $\Pi = 1 \otimes \tau_x$ , instead of  $1 \otimes \tau_z$ , then how would the parities in the column  $\Pi \Gamma \Pi^{-1}$  of Table I be changed?

2. Show that, given the unitary matrix,

$$U(x) = e^{\frac{i}{2}\theta_1\sigma_3} e^{\frac{i}{2}\theta_2\sigma_2} e^{\frac{i}{2}\theta_3\sigma_3}, \quad (1.107)$$

where  $\theta_1, \theta_2, \theta_3$  are the Euler angles, one has,

$$\text{tr}(U^\dagger \partial_1 U U^\dagger \partial_2 U U^\dagger \partial_3 U) = \frac{1}{4} \sin \theta_2. \quad (1.108)$$

3. With the help of Eq. (1.101), and given

$$H(\mathbf{k}) = \mathbf{h}(\mathbf{k}) \cdot \vec{\Gamma}, \quad (1.109)$$

where  $\Gamma_a$  are the 5 generators of the Clifford algebra, show that, for the two energy branches,

$$C_2 = \pm \frac{3}{8\pi^2} \int_{BZ} d^4 k \epsilon_{abcde} \hat{h}_a \partial_1 \hat{h}_b \partial_2 \hat{h}_c \partial_3 \hat{h}_d \partial_4 \hat{h}_e. \quad (1.110)$$

### References

- Avron, J. E., L. Sadun, J. Segert, and B. Simon, 1988, Phys. Rev. Lett. **61**, 1329.
- Avron, J. E., L. Sadun, J. Segert, and B. Simon, 1989, Communications in Mathematical Physics **124**(4), 595.
- Bernevig, B. A., and T. L. Hughes, 2013, *Topological Insulators and Topological Superconductors* (Princeton University Press).
- Coleman, S., 1985, *Aspects of Symmetry: Selected Erice Lectures* (Cambridge University Press).
- Dittrich, W., and M. Reuter, 1986, *Selected Topics in Gauge Theories*, volume 244 of *Lecture Notes in Physics* (Springer-Verlag).
- Gottfried, K., 1989, *Quantum mechanics* (Addison-Wesley).
- Murakami, S., N. Nagaosa, and S.-C. Zhang, 2004, Phys. Rev. B **69**, 235206.
- Ryu, S., A. P. Schnyder, A. Furusaki, and A. W. W. Ludwig, 2010, New Journal of Physics **12**(6), 065010.
- Soluyanov, A. A., and D. Vanderbilt, 2012, Phys. Rev. B **85**, 115415.