Memo: Spin Space Groups

Ken Shiozaki

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Abstract

These are notes on spin space groups.

1 Generalities on crystalline symmetries

The treatment here includes arbitrary crystalline symmetries, such as magnetic space groups, spin space groups, and magnetic translation groups.

Let G be a crystalline symmetry group. For each $g \in G$, let $p_g \in O(3)$ be the rotation matrix and $\boldsymbol{t}_g \in \mathbb{R}^3$ be the translation vector, and write the left action of G on real space $\mathbb{R}^3$ as

$$g(\boldsymbol{r}) = p_g \boldsymbol{r} + \boldsymbol{t}_g, \quad g \in G, \boldsymbol{r} \in \mathbb{R}^d. \tag{1.1}$$

From the group structure of G,

$$\boldsymbol{t}_g + p_g \boldsymbol{t}_h = \boldsymbol{t}_{gh}, \quad g, h \in G, \tag{1.2}$$

holds. We consider the action of G on a Hilbert space. Let

$$\phi : G \to \mathbb{Z}_2 = \{\pm 1\} \tag{1.3}$$

be the homomorphism specifying whether each element of G is unitary or antiunitary. We denote the action on the Hilbert space by $\hat{g}$. The $U(1)$-valued factor system $z_{g,h}$ is defined by

$$\hat{g}\hat{h} = z_{g,h}\widehat{gh}, \quad g, h \in G. \tag{1.4}$$

The two decompositions of $\widehat{ghl}$ give the cocycle condition

$$(\delta z)_{g,h,l} = z_{h,l}^{\phi_g} z_{gh,l}^{-1} z_{g,hl} z_{g,h}^{-1} = 1, \quad g, h, l \in G. \tag{1.5}$$

The redefinition

$$\hat{g} \mapsto \eta_g \hat{g}, \quad \eta_g \in U(1) \tag{1.6}$$

changes $z_{g,h}$ as

$$z_{g,h} \mapsto z_{g,h} \times (\delta\eta)_{g,h}, \quad (\delta\eta)_{g,h} = \eta_h^{\phi_g} \eta_{gh}^{-1} \eta_g, \quad g, h \in G. \tag{1.7}$$

This induces the equivalence relation $z \sim z\delta\eta$. The equivalence class $[z]$ belongs to the group cohomology $H^2(G, U(1)_\phi)$.

In the problem of topological invariants and the classification of topological insulators and superconductors, the input data are

- the group G,
- the action on real space $g(\boldsymbol{r}) = p_g \boldsymbol{r} + \boldsymbol{t}_g$,
- the homomorphism ϕ specifying unitary/antiunitary character,
- the cohomology class $[z]$ of the factor system.

Once these data are fixed, a K-group is defined. If the K-group can be computed through the Atiyah-Hirzebruch spectral sequence [1], one obtains how many definable topological invariants there are, somewhat explicit formulae for them, and the classification of possible boundary states, including surface, hinge, and corner states.

1.1 How to specify the data

Since the group G itself contains infinitely many elements, we describe the structure of G by focusing on the finite point group. The method is as follows. Define the translation group Π by

$$\Pi = \{g \in G | p_g = \mathbb{1}, \phi_g = 1, z_{g,h} = 1 \text{ for all } h \in G\}. \tag{1.8}$$

Notice that this definition depends on the ambiguity in the factor system $z_{g,h}$. For example, in a magnetic translation group, $z_{g,h}$ depends on the gauge. The group Π is an abelian normal subgroup of G, and

$$P := G/\Pi \tag{1.9}$$

is called the point group. Note the short exact sequence

$$0 \to \Pi \to G \xrightarrow{\pi} P \to 0. \tag{1.10}$$

A map

$$s : P \to G \tag{1.11}$$

is called a section when $\pi \circ s = \mathrm{id}$ holds. Since P is finite, specifying a section $s : P \to G$ gives the crystalline group G concretely. The point group P is isomorphic to the direct product of some crystallographic point group and a finite group. We label the elements of the point group P by integers $j = 1, \dots, |P|$, and simply write the product in P as ij. By definition,

$$s_j(\boldsymbol{r}) = p_{s_j} \boldsymbol{r} + \boldsymbol{t}_{s_j}, \tag{1.12}$$

so for each point-group element $j \in P$ we obtain a rotation matrix p_{s_j} and a translation vector $\boldsymbol{t}_{s_j}$. We write

$$p_j := p_{s_j}, \quad \boldsymbol{t}_j := \boldsymbol{t}_{s_j}, \quad j = 1, \dots, |P|. \tag{1.13}$$

By the definition of a section,

$$s_i s_j \equiv s_{ij} \mod \Pi, \tag{1.14}$$

that is,

$$p_i p_j = p_{ij}, \quad p_i \boldsymbol{t}_j + \boldsymbol{t}_i - \boldsymbol{t}_{ij} \in \{\text{lattice vectors}\}. \tag{1.15}$$

The section has the ambiguity

$$s_j \mapsto s_j a = a s_j, \quad a \in \Pi, \tag{1.16}$$

but since $\phi(\Pi) = 1$ by the definition of the translation group Π, the homomorphism on the point group,

$$\phi_i := \phi_{s_i}, \tag{1.17}$$

is well-defined. For the factor system, the cocycle condition gives, for $g, h \in G$ and $a \in \Pi$,

$$(\delta z)_{g,h,a} = z_{h,a}^{\phi_g} z_{gh,a}^{-1} z_{g,ha} z_{g,h}^{-1} = z_{g,ha} z_{g,h}^{-1} = 1, \tag{1.18}$$
$$(\delta z)_{a,g,h} = z_{g,h}^{\phi_a} z_{ag,h}^{-1} z_{a,gh} z_{a,g}^{-1} = z_{g,h} z_{ag,h}^{-1} = 1. \tag{1.19}$$

Therefore the point-group factor system

$$z_{i,j} := z_{s_i,s_j}, \quad i,j \in P \tag{1.20}$$

does not depend on the choice of section s.

In summary, to specify a crystalline symmetry, it is enough to give the following data for the finite point group P:

- lattice vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$,
- the multiplication table $(i,j) \mapsto ij$ of the finite group P,
- rotation matrices $p_j \in O(3)$,
- translation vectors $\boldsymbol{t}_j \in \mathbb{R}^3$,
- the homomorphism ϕ_j,
- the factor system $\{z_{i,j}\}_{i,j \in P}$.

The computational implementation of the Atiyah-Hirzebruch spectral sequence in Ref. [1] can compute up to the E_2 page once these data are given, independently of the type of symmetry.

2 Classification problem for spin space groups

Here we consider space groups. In other words, both ϕ and the factor system z are assumed to be trivial. Let G be a space group. As notation, let

$$P_G = \{p_g | g \in G\}, \tag{2.1}$$
$$L_G = \{\boldsymbol{t}_g | p_g = 1, g \in G\} \tag{2.2}$$

denote respectively the group of $O(3)$ rotation matrices and the group of translation vectors of the space group. Repeated elements are not counted. Then

$$pL_G = L_G, \quad p \in P_G \tag{2.3}$$

holds.

Given a space group G and a spin group, or spin-only group, $B \subset O(3)$, define a spin space group $X \subset G \times O(3)$ as a subgroup satisfying the following two conditions:

$$\{\, g \mid (g,u) \in X \,\} = G, \tag{2.4}$$
$$\{\, u \mid (g,u) \in X \,\} = B. \tag{2.5}$$

The goal is to give a method to enumerate all groups X satisfying (2.4) and (2.5). In particular, we are interested in classifying independent spin space groups after identifying those that are equivalent under conjugation in $G \times O(3)$. Thus we would like to obtain the equivalence classes under

$$X \sim (h,v)X(h,v)^{-1} = \{\, (hgh^{-1}, vuv^\top) \mid (g,u) \in X \,\}, \qquad (h,v) \in G \times O(3). \tag{2.6}$$

- For example, if $G = \mathbb{Z} = \{t_n | n \in \mathbb{Z}\}$ is the one-dimensional translation group and $B = \mathbb{Z}_n = \langle c | c^n \rangle$, then examples include

$$X = \{(1, t_n, c^n) | n \in \mathbb{Z}\}, \tag{2.7}$$

$$X = \{(1, t_n, c^m) | n \in \mathbb{Z}, m \in \mathbb{Z}/n\} = G \times B. \tag{2.8}$$

By Goursat's lemma, recalled in App. A, spin space groups X are in one-to-one correspondence with triples

$$(N_G \triangleleft G, N_B \triangleleft B, \theta : G/N_G \xrightarrow{\cong} B/N_B). \tag{2.9}$$

Therefore the problem decomposes into the following four steps:

(i) classify the normal subgroups N_G of the space group G,

(ii) classify the normal subgroups N_B of the spin group B,

(iii) classify the isomorphisms $G/N_G \xrightarrow{\cong} B/N_B$,

(iv) quotient by the conjugation relation (2.6).

Note that the third condition restricts the pair of normal subgroups N_G, N_B to those satisfying the group isomorphism $G/N_G \cong B/N_B$.

Below I record notes on the construction of normal subgroups of a space group.

2.1 Normal subgroups of a space group

We specify the space group G by the following data:

- Lattice vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$. Namely, $L_G = \{\sum_{l=1}^{3} n_l \boldsymbol{a}_l | n_l \in \mathbb{Z}\}$.
- The multiplication table $(i, j) \mapsto ij$ of the label set $P_G = \{1, \ldots, |P_G|\}$.
- The point-group rotation matrices $\{p_i \in O(3)\}_{i \in P_G}$, with $p_1 = \mathbb{1}$.
- The translation vectors $\{\boldsymbol{t}_i \in \mathbb{R}^3\}_{i \in P_G}$, with $\boldsymbol{t}_1 = \boldsymbol{0}$.

The projection of $\boldsymbol{t}_i$ to its value modulo L_G is a representative 1-cocycle of the group cohomology class characterizing the extension (1.10):

$$\boldsymbol{t}_i \bmod L_G \in Z^1(P_G, \mathbb{R}^3/L_G), \quad [\boldsymbol{t} \bmod L_G] \in H^1(P_G, \mathbb{R}^3/L_G) \cong H^2(P_G, L_G). \tag{2.10}$$

Here

$$\boldsymbol{\omega}_{i,j} = (\delta \boldsymbol{t})_{i,j} = p_i \boldsymbol{t}_j + \boldsymbol{t}_i - \boldsymbol{t}_{ij} \in L_G \tag{2.11}$$

is the Bockstein homomorphism

$$H^1(P_G, \mathbb{R}^3/L_G) \to H^2(P_G, L_G), \quad [\boldsymbol{t} \bmod L_G] \mapsto [\boldsymbol{\omega}].$$

Write the translation group and point group of a normal subgroup $N \triangleleft G$ as

$$1 \to \Pi_N \to N \to P_N \to 1, \tag{2.12}$$

respectively. We also write the corresponding sets of lattice vectors as

$$L_G = \{\boldsymbol{t}_g | g \in \Pi_G\}, \tag{2.13}$$
$$L_N = \{\boldsymbol{t}_g | g \in \Pi_N\}. \tag{2.14}$$

Write an element of the space group in Seitz notation[1] as

$$g = \{p_g | \boldsymbol{t}_g\}. \tag{2.15}$$

Its inverse is

$$g^{-1} = \{p_g^{-1} | -p_g^{-1}\boldsymbol{t}_g\}. \tag{2.16}$$

The condition that a subgroup $N \subset G$ is normal is that, for any $n \in N$ and $g \in G$,

$$\begin{aligned} gng^{-1} &= \{p_g|\boldsymbol{t}_g\}\{p_n|\boldsymbol{t}_n\}\{p_g^{-1}| - p_g^{-1}\boldsymbol{t}_g\} && (2.17)\\ &= \{p_g|\boldsymbol{t}_g\}\{p_n p_g^{-1}| - p_n p_g^{-1}\boldsymbol{t}_g + \boldsymbol{t}_n\} && (2.18)\\ &= \{p_g p_n p_g^{-1}|p_g(-p_n p_g^{-1}\boldsymbol{t}_g + \boldsymbol{t}_n) + \boldsymbol{t}_g\} && (2.19)\\ &= \{p_{gng^{-1}}|p_g\boldsymbol{t}_n - p_{gng^{-1}}\boldsymbol{t}_g + \boldsymbol{t}_g\} \in N. && (2.20) \end{aligned}$$

This gives the following two necessary conditions:

- $P_N \lhd P_G$.
- $P_G(L_N) = L_N$.

The latter is obtained by restricting to $n \in \Pi_N$. We call a sublattice $L' \in L_G$ satisfying $P_G(L') = L'$ a P_G-invariant sublattice. For a given normal subgroup $P_N \lhd P_G$ and a P_G-invariant sublattice $L_N \subset L_G$, $P_G(L_N) = L_N$, we derive the condition under which the space group N constructed by a section $s' : P_N \to N$ becomes a normal subgroup $N \lhd G$.

Represent the normal subgroup $P_N \lhd P_G$ as a subset of the label set, $P_N \subset \{1, \dots, |P_G|\}$. That is,

$$i\sigma i^{-1} \in P_N, \quad i \in P_G, \quad \sigma \in P_N \tag{2.21}$$

holds. Let $\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3$ be lattice vectors of the P_G-invariant sublattice L_N. Then

$$p_i\boldsymbol{b}_l \in L_N, \quad i \in P_G, \quad l \in \{1, 2, 3\} \tag{2.22}$$

holds. Since an element of the space group G is written uniquely as $\{p_i|\boldsymbol{t}_i + \boldsymbol{u}\}$ with $\boldsymbol{u} \in L_G$, a section $s' : P_N \to N$ characterizing the subgroup $N \subset G$ can be written as

$$s'_\sigma = \{p_\sigma|\boldsymbol{t}_\sigma + \boldsymbol{u}_\sigma\}, \quad \boldsymbol{u} \in C^1(P_N, L_G). \tag{2.23}$$

Note that the ambiguity of $\boldsymbol{u}_\sigma$ by elements of L_N gives the same space group N. Possible 1-cochains $\boldsymbol{u}$ are constrained by the cocycle condition for $\boldsymbol{t}_\sigma + \boldsymbol{u}_\sigma$:

$$p_\rho(\boldsymbol{t}_\sigma + \boldsymbol{u}_\sigma) + (\boldsymbol{t}_\rho + \boldsymbol{u}_\rho) - (\boldsymbol{t}_{\rho\sigma} + \boldsymbol{u}_{\rho\sigma}) = \boldsymbol{\omega}_{\rho,\sigma} + (\delta\boldsymbol{u})_{\rho,\sigma} \in L_N, \quad \rho, \sigma \in P_N. \tag{2.24}$$

Therefore the 1-cochain $\boldsymbol{u} \in C^1(P_N, L_G)$ is a solution of the linear equation

$$\delta\boldsymbol{u} = -\boldsymbol{\omega}|_{P_N} \bmod L_N. \tag{2.25}$$

Using this solution $\boldsymbol{u}$, a 2-cocycle $\boldsymbol{\omega}' \in Z^2(P_N, L_N)$ is obtained as

$$\boldsymbol{\omega}' = \boldsymbol{\omega}|_{P_N} + \delta\boldsymbol{u}. \tag{2.26}$$

[1] A faithful representation.

Next, we find the condition that the section s' gives a normal subgroup $N \lhd G$. Comparing

$$s_i s'_\sigma s_i^{-1} = \{p_i p_\sigma p_i^{-1} | p_i(-p_\sigma p_{i^{-1}} \boldsymbol{t}_i + \boldsymbol{t}_\sigma + \boldsymbol{u}_\sigma) + \boldsymbol{t}_i\} \tag{2.27}$$

$$= \{p_{i\sigma i^{-1}} | p_i(\boldsymbol{t}_\sigma + \boldsymbol{u}_\sigma) - p_{i\sigma i^{-1}} \boldsymbol{t}_i + \boldsymbol{t}_i\}, \tag{2.28}$$

with

$$s'_{i\sigma i^{-1}} = \{p_{i\sigma i^{-1}} | \boldsymbol{t}_{i\sigma i^{-1}} + \boldsymbol{u}_{i\sigma i^{-1}}\}, \tag{2.29}$$

we obtain the linear equation for $\boldsymbol{u}_\sigma$:

$$p_i \boldsymbol{u}_\sigma - \boldsymbol{u}_{i\sigma i^{-1}} \equiv -\boldsymbol{t}_i + p_{i\sigma i^{-1}} \boldsymbol{t}_i - p_i \boldsymbol{t}_\sigma + \boldsymbol{t}_{i\sigma i^{-1}} \tag{2.30}$$

$$\equiv -(p_i \boldsymbol{t}_\sigma + \boldsymbol{t}_i - \boldsymbol{t}_{i\sigma}) + (p_{i\sigma i^{-1}} \boldsymbol{t}_i + \boldsymbol{t}_{i\sigma i^{-1}} - \boldsymbol{t}_{i\sigma}) \tag{2.31}$$

$$\equiv -\boldsymbol{\omega}_{i,\sigma} + \boldsymbol{\omega}_{i\sigma i^{-1},i} \bmod L_N, \quad i \in P_G, \sigma \in P_N. \tag{2.32}$$

The result is summarized as follows.

Normal subgroups $N \lhd G$ of a space group G are obtained by the following procedure.

- Choose a normal subgroup $P_N \lhd P_G$ of the point group.
- Choose a P_G-invariant subgroup $L_N \subset L_G$ of the translation group, satisfying $P_G(L_N) = L_N$.
- Solve the following linear equations for the unknowns $\{\boldsymbol{u}_\sigma \in L_G\}_{\sigma \in P_N}$:

$$\begin{cases} p_\rho \boldsymbol{u}_\sigma + \boldsymbol{u}_\rho - \boldsymbol{u}_{\rho\sigma} \equiv -p_\rho \boldsymbol{t}_\sigma + \boldsymbol{t}_\rho - \boldsymbol{t}_{\rho\sigma} \bmod L_N, & \rho, \sigma \in P_N, \\ p_i \boldsymbol{u}_\sigma - \boldsymbol{u}_{i\sigma i^{-1}} \equiv -\boldsymbol{t}_i + p_{i\sigma i^{-1}} \boldsymbol{t}_i - p_i \boldsymbol{t}_\sigma + \boldsymbol{t}_{i\sigma i^{-1}} \bmod L_N, & i \in P_G, \sigma \in P_N. \end{cases} \tag{2.33}$$

2.1.1 Note on solving (2.33)

The equation (2.33) is solved explicitly as follows. Expand $\boldsymbol{u}_i$ in the lattice vectors of L_G:

$$\boldsymbol{u}_i = \sum_j x_{ij} \boldsymbol{a}_j, \quad x_{ij} \in \mathbb{Z}, i \in P_N, \tag{2.34}$$

$$X = (x_{ij})_{i \in P_N, j=1,2,3}. \tag{2.35}$$

Then (2.33) takes the form

$$AX \equiv B \bmod L_N. \tag{2.36}$$

Using a generalized inverse matrix A^+ of A, one solution over the rational numbers is obtained as

$$X \equiv A^+ B. \tag{2.37}$$

If the resulting X is integral, it is a solution. If X is not integral, one has to examine whether there is no integral solution, or whether an integral solution should be searched for by using the freedom modulo L_N. It would be efficient to check this point during implementation.

2.1.2 Structure of the quotient group G/N

The quotient group G/N fits into the following exact sequence; see App. B for the proof:

$$1 \to L_G/L_N \to G/N \to P_G/P_N \to 1. \tag{2.38}$$

Therefore the group structure of G/N is determined once the 2-cocycle $Z^2(P_G/P_N, L_G/L_N)$ characterizing the extension is determined.

Let

$$P_G/P_N \to P_G, \quad a \mapsto i_a, \quad i_1 = 1 \tag{2.39}$$

be a complete set of representatives of P_G/P_N. Then

$$P_G = \bigcup_{a \in P_G/P_N} i_a P_N. \tag{2.40}$$

Define $t_{a,b}$ by the relation

$$i_a i_b = i_{ab} t_{a,b}, \quad t_{a,b} \in P_N. \tag{2.41}$$

From the general theory in App. B, the 2-cocycle $\bar{\boldsymbol{\omega}}_{a,b}$ is given by

$$\bar{\boldsymbol{\omega}}_{a,b} \equiv \boldsymbol{\omega}_{i_a,i_b} + \boldsymbol{\omega}_{t_{a,b},i_{ab}} - \boldsymbol{u}_{t_{a,b}} \bmod L_N. \tag{2.42}$$

Thus the group structure of G/N is determined as

$$(a, \boldsymbol{\tau})(b, \boldsymbol{\tau}') = (ab, p_a \boldsymbol{\tau}' + \boldsymbol{\tau} + \bar{\boldsymbol{\omega}}_{a,b}), \quad (a, \boldsymbol{\tau}), (b, \boldsymbol{\tau}') \in P_G/P_N \times L_G/L_N. \tag{2.43}$$

2.2 Normal subgroups of the spin group

The problem of finding normal subgroups $N_B \lhd B$ of a given spin group B is simply the problem of finding normal subgroups of a finite group, so we do not discuss it here.

2.3 Isomorphisms $\theta : G/N_G \xrightarrow{\cong} B/N_B$

This is left for later.

3 Coupling terms to spin

Let us express a magnetic structure in real space by a three-dimensional vector field

$$\boldsymbol{M}(\boldsymbol{r}) = (M_x(\boldsymbol{r}), M_y(\boldsymbol{r}), M_z(\boldsymbol{r}))^\top, \quad \boldsymbol{r} \in \mathbb{R}^3. \tag{3.1}$$

Consider the situation where this vector field satisfies the symmetry

$$\boldsymbol{M}(g\boldsymbol{r}) = O_g \boldsymbol{M}(\boldsymbol{r}), \quad O_g \in O(3), \quad g \in G, \tag{3.2}$$

$$O_g O_h = O_{gh}, \quad g, h \in G. \tag{3.3}$$

Let $R_{\hat{n},\theta}$ denote the $SO(3)$ matrix for a rotation by angle θ about the direction $\hat{n}$, and let

$$I = \mathrm{diag}(-1, -1, -1)$$

be the inversion matrix. Writing the three Pauli matrices as the vector

$$\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)^\top, \tag{3.4}$$

we note that

$$e^{-i\theta\sigma_z/2}\boldsymbol{\sigma}e^{i\theta\sigma_z/2} = (\sigma_x e^{i\theta\sigma_z}, \sigma_y e^{i\theta\sigma_z}, \sigma_z)^\top \tag{3.5}$$

$$= (\sigma_x\cos\theta + \sigma_y\sin\theta, \sigma_y\cos\theta - \sigma_x\sin\theta, \sigma_z)^\top \tag{3.6}$$

$$= \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \boldsymbol{\sigma} = R^\top_{\hat{z},\theta}\boldsymbol{\sigma} \tag{3.7}$$

and

$$\sigma_y\boldsymbol{\sigma}^*\sigma_y = -\boldsymbol{\sigma} = I\boldsymbol{\sigma}. \tag{3.8}$$

Write an orthogonal matrix $O_g \in O(3)$ as

$$O_g = R_{\hat{n}_g,\theta_g} I^{\frac{1-\det O_g}{2}}. \tag{3.9}$$

Then

$$O_g^\top\boldsymbol{\sigma} = I^{\frac{1-\det O_g}{2}} R^\top_{\hat{n}_g,\theta_g}\boldsymbol{\sigma} = I^{\frac{1-\det O_g}{2}} e^{-i\theta_g\hat{n}_g\cdot\boldsymbol{\sigma}/2}\boldsymbol{\sigma}e^{i\theta_g\hat{n}_g\cdot\boldsymbol{\sigma}/2} \tag{3.10}$$

$$= \begin{cases} e^{-i\theta_g\hat{n}_g\cdot\boldsymbol{\sigma}/2}\boldsymbol{\sigma}e^{i\theta_g\hat{n}_g\cdot\boldsymbol{\sigma}/2} & (\det O_g = 1) \\ e^{-i\theta_g\hat{n}_g\cdot\boldsymbol{\sigma}/2}\sigma_y\boldsymbol{\sigma}^*\sigma_y e^{i\theta_g\hat{n}_g\cdot\boldsymbol{\sigma}/2} & (\det O_g = -1) \end{cases} \tag{3.11}$$

follows. Therefore the symmetry of the coupling term to the spin operator can be written as

$$\boldsymbol{M}(g\boldsymbol{r})^\top\boldsymbol{\sigma} = \hat{u}_g(\boldsymbol{M}(\boldsymbol{r})^\top\boldsymbol{\sigma})\hat{u}_g^{-1}, \quad \hat{u}_g = e^{-i\theta_g\hat{n}_g\boldsymbol{\sigma}/2}(\sigma_y K)^{\frac{1-\det O_g}{2}}, \quad g \in G, \tag{3.12}$$

where K denotes complex conjugation.

The factor system obeyed by $\hat{u}_g$ is

$$\hat{u}_g\hat{u}_h = e^{-i\theta_g\hat{n}_g\boldsymbol{\sigma}/2}(\sigma_y K)^{\frac{1-\det O_g}{2}} e^{-i\theta_h\hat{n}_h\boldsymbol{\sigma}/2}(\sigma_y K)^{\frac{1-\det O_h}{2}} \tag{3.13}$$

$$= e^{-i\theta_g\hat{n}_g\boldsymbol{\sigma}/2}e^{-i\theta_h\hat{n}_h\boldsymbol{\sigma}/2}(\sigma_y K)^{\frac{1-\det O_g}{2}}(\sigma_y K)^{\frac{1-\det O_h}{2}} \tag{3.14}$$

$$= z^{\rm sp}_{g,h}(-1)^{\frac{1-\det O_g}{2}\frac{1-\det O_h}{2}} \times \hat{u}_{gh}. \tag{3.15}$$

Here we have set

$$z^{\rm sp}_{g,h} = \begin{cases} 1 & (e^{-i\theta_g\hat{n}_g\boldsymbol{\sigma}/2}e^{-i\theta_h\hat{n}_h\boldsymbol{\sigma}/2} = e^{-i\theta_{gh}\hat{n}_{gh}\boldsymbol{\sigma}/2}), \\ -1 & (e^{-i\theta_g\hat{n}_g\boldsymbol{\sigma}/2}e^{-i\theta_h\hat{n}_h\boldsymbol{\sigma}/2} = -e^{-i\theta_{gh}\hat{n}_{gh}\boldsymbol{\sigma}/2}). \end{cases} \tag{3.16}$$

Thus, in a numerical computation, it is enough to set

$$R_g = \begin{cases} O_g & (\det O_g = 1), \\ O_g I & (\det O_g = -1), \end{cases} \tag{3.17}$$

choose one lift

$$R_g \mapsto \tilde{R}_g \in {\rm Spin}(3), \quad g \in G, \tag{3.18}$$

and then compute

$$z^{\rm sp}_{g,h} = \tilde{R}_g\tilde{R}_h\tilde{R}^\dagger_{gh}. \tag{3.19}$$

A Goursat's lemma

For Goursat's lemma, Ref. [2] is a useful reference. We write the identity element of a group as e. In general, for a group homomorphism $f : A \to B$ and a subgroup $S \subset B$, note that

$$f^{-1}(S) = \{a \in A | f(a) \in S\}$$

is a group. Indeed, if $a, a' \in f^{-1}(S)$, then $aa' \in f^{-1}(S)$ because $f(aa') = f(a)f(a') \in S$.

Lemma A.1 (Goursat)**.** *Let A, B be groups. There is a one-to-one correspondence between subgroups $C \subset A \times B$ and quintuples $Q = (\bar{A}, N_A, \bar{B}, N_B, \theta)$. Here $N_A \lhd \bar{A} \subset A$, $N_B \lhd \bar{B} \subset B$, and θ is an isomorphism*

$$\theta : \bar{A}/N_A \xrightarrow{\cong} \bar{B}/N_B.$$

Proof following Ref. [2]. Let C be a subgroup $C \subset A \times B$. Define

$$\bar{A} = \{a \in A | (a, b) \in C\}, \quad N_A = \{a \in A | (a, e) \in C\}, \tag{A.1}$$

$$\bar{B} = \{b \in B | (a, b) \in C\}, \quad N_B = \{b \in B | (e, b) \in C\}. \tag{A.2}$$

Since C is a group, $\bar{A}$ and $\bar{B}$ are also groups. For any $a' \in N_A$ and $a \in \bar{A}$, there exists $b \in B$ such that

$$(a, b)(a', e)(a, b)^{-1} = (aa'a^{-1}, e), \tag{A.3}$$

and hence $aN_Aa^{-1} = N_A$. Thus $N_A \lhd \bar{A}$. Similarly, $N_B \lhd \bar{B}$. Define θ by

$$\theta(aN_A) := bN_B, \quad \text{where } (a, b) \in C. \tag{A.4}$$

The right-hand side is well-defined as follows. If $(a, b), (a, b') \in C$, then $(a, b)^{-1}(a, b') = (1, b^{-1}b') \in C$, so $b^{-1}b' \in N_B$, equivalently $b \in b'N_B$. Similarly, if $(a, b), (a', b) \in C$, then $a \in a'N_A$, so the left-hand side is also well-defined. The homomorphism property follows from the fact that if $(a, b), (a', b') \in C$, then $(a, b)(a', b') = (aa', bb') \in C$. If $\theta(a) = N_B$, then $(a, b) \in C$ and $(e, b) \in C$. Then $(a, e) = (a, b)(e, b)^{-1} \in C$, so $a \in N_A$; hence θ is injective. For any $b \in \bar{B}$, there exists a such that $(a, b) \in C$, so θ is surjective. This constructs the quintuple $f(C) := (\bar{A}, N_A, \bar{B}, N_B, \theta)$.

Conversely, given a quintuple $Q = (\bar{A}, N_A, \bar{B}, N_B, \theta)$, define the subset

$$\mathcal{G}_\theta := \{(aN_A, \theta(aN_A)) | aN_A \in \bar{A}/N_A\} \subset \bar{A}/N_A \times \bar{B}/N_B. \tag{A.5}$$

By the homomorphism property of θ, $\mathcal{G}_\theta$ is a group. Taking the inverse image under the natural surjection

$$p : \bar{A} \times \bar{B} \to \bar{A}/N_A \times \bar{B}/N_B, \tag{A.6}$$

we obtain the subgroup

$$g(Q) := p^{-1}(\mathcal{G}_\theta) \subset \bar{A} \times \bar{B} \subset A \times B. \tag{A.7}$$

Finally, we show that these two correspondences are inverse to each other.

First, we show $g \circ f = \mathrm{id}$. Let $C \subset A \times B$ be a subgroup, and let $f(C) = (\bar{A}, N_A, \bar{B}, N_B, \theta)$ be as above. Then

$$g(f(C)) = \{\, (a, b) \in A \times B \mid (aN_A,\ bN_B) \in \mathcal{G}_\theta \,\}. \tag{A.8}$$

By the definition of $\mathcal{G}_\theta$,

$$(aN_A,\ bN_B) \in \mathcal{G}_\theta \iff (a, b) \in C, \tag{A.9}$$

and therefore $g(f(C)) = C$.

Next, we show $f \circ g = \mathrm{id}$. Given $Q = (\bar{A}, N_A, \bar{B}, N_B, \theta)$, set $C' := g(Q) = p^{-1}(\mathcal{G}_\theta) \subset \bar{A} \times \bar{B}$. Construct $f(C') = (\bar{A}', N_A', \bar{B}', N_B', \theta')$ from C'. First,

$$\bar{A}' = \{\, a \in A \mid (a,b) \in C' \,\} = \{\, a \in A \mid a \in \bar{A} \,\} = \bar{A}, \tag{A.10}$$

$$\bar{B}' = \{\, b \in B \mid (a,b) \in C' \,\} = \{\, b \in B \mid bN_B \in \theta(\bar{A}/N_A) = \bar{B}/N_B \,\} = \{\, b \in B \mid b \in \bar{B} \,\} = \bar{B}, \tag{A.11}$$

$$N_A' = \{\, a \in A \mid (a,e) \in C' \,\} = \{\, a \in A \mid \theta(aN_A) = N_B \,\} = \{\, a \in A \mid a \in N_A \,\} = N_A, \tag{A.12}$$

$$N_B' = \{\, b \in B \mid (e,b) \in C' \,\} = \{\, b \in B \mid bN_B = \theta(N_A) = N_B \,\} = \{\, b \in B \mid b \in N_B \,\} = N_B. \tag{A.13}$$

It remains to show $\theta' = \theta$. By definition,

$$\theta'(aN_A) = bN_B, \quad \text{where } (a,b) \in C', \tag{A.14}$$

but $(a,b) \in C'$ is equivalent to $a \in \bar{A}$ and $bN_B = \theta(aN_A)$. Thus $\theta' = \theta$. □

B Exact sequence for a quotient group

Proposition B.1. *Given an exact sequence of groups*

$$1 \to A \xrightarrow{i} G \xrightarrow{\pi} Q \to 1 \tag{B.1}$$

and a normal subgroup $N \lhd G$, there is an exact sequence

$$1 \to A/(A \cap N) \xrightarrow{\iota} G/N \xrightarrow{\bar{\pi}} Q/\pi(N) \to 1. \tag{B.2}$$

Here

$$\iota(a(A \cap N)) = i(a)N, \tag{B.3}$$
$$\bar{\pi}(gN) := \pi(g)\pi(N). \tag{B.4}$$

Note the third isomorphism theorem $AN/N \cong A/(A \cap N)$.

Proof. The subgroup $A \cap N$ is normal in A, since if $n \in A \cap N$, then $ana^{-1} \in N$ and $ana^{-1} \in A$. The map ι is well-defined because if $a(A \cap N) = a'(A \cap N)$, then $a^{-1}a' \in A \cap N$. The injectivity of ι follows from the fact that if $a \in A$ and $i(a)N = N$, then $i(a) \in N$, so $a \in A \cap N$.

The subgroup $\pi(N)$ is normal in Q: for $q \in Q$, write $q = \pi(g)$; then

$$q\pi(n)q^{-1} = \pi(gng^{-1}) \in \pi(N).$$

The map $\bar{\pi}$ is well-defined because if $gN = g'N$, then $g^{-1}g' \in N$, and hence

$$\pi(g')\pi(N) = \pi(g)\pi(g^{-1}g')\pi(N) = \pi(g)\pi(N).$$

It is a homomorphism, and it is surjective because π is surjective.

The inclusion $\operatorname{im}\iota \subset \ker\bar{\pi}$ follows from

$$\bar{\pi}(i(a)N) = \pi(i(a))\pi(N) = \pi(N).$$

Conversely, suppose $gN \in \ker \bar{\pi}$. Then $\pi(g)\pi(N) = \pi(N)$, so $\pi(g) \in \pi(N)$. Thus there is $n \in N$ such that $\pi(g) = \pi(n)$. Hence $\pi(gn^{-1}) = e$, so $gn^{-1} \in \ker \pi = \operatorname{im} i$. Therefore $g \in i(a)N$ for some $a \in A$, and gN lies in $\operatorname{im} \iota$. □

Let A be an abelian group. We construct the group structure of G/N from the information of sections

$$s : Q \to G, \quad s_1 = 1, \tag{B.5}$$
$$u : \pi(N) \to N, \quad u_1 = 1. \tag{B.6}$$

Let the 2-cocycle determined by the section s be

$$\omega_{p,q} := s_p s_q s_{pq}^{-1} \in A, \quad \omega \in Z^2(Q, A). \tag{B.7}$$

Choose representatives

$$r : Q/\pi(N) \to Q, \quad r_1 = 1, \tag{B.8}$$

and define

$$t_{x,y} := r_x r_y r_{xy}^{-1} \in \pi(N). \tag{B.9}$$

Then define

$$\sigma : Q/\pi(N) \to G/N, \quad \sigma_x := s_{r_x} N. \tag{B.10}$$

The corresponding 2-cocycle is obtained from

$$\begin{aligned} \sigma_x \sigma_y &= s_{r_x} N s_{r_y} N = s_{r_x} s_{r_y} N = \omega_{r_x, r_y} s_{r_x r_y} N = \omega_{r_x, r_y} s_{t_{x,y} r_{xy}} N && \text{(B.11)} \\ &= \omega_{r_x, r_y} \omega_{t_{x,y}, r_{xy}} s_{t_{x,y}} s_{r_{xy}} N = \omega_{r_x, r_y} \omega_{t_{x,y}, r_{xy}} s_{t_{x,y}} N \sigma_{xy} && \text{(B.12)} \\ &= \omega_{r_x, r_y} \omega_{t_{x,y}, r_{xy}} s_{t_{x,y}} u_{t_{x,y}}^{-1} N \sigma_{xy}. && \text{(B.13)} \end{aligned}$$

Here we used

$$\pi(s_x u_x^{-1}) = \pi(s_x)\pi(u_x^{-1}) = x x^{-1} = e, \tag{B.14}$$

so $s_x u_x^{-1} \in \ker \pi = A$. Thus the 2-cocycle

$$\bar{\omega}_{x,y} = \omega_{r_x, r_y} \omega_{t_{x,y}, r_{xy}} s_{t_{x,y}} u_{t_{x,y}}^{-1} N \in AN/N \tag{B.15}$$

is determined.

The independence of the cohomology class from the choices of representatives r and sections s, u is left for later.

References

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