Space Groups and Their Representations by Prof. Yang Qi

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1 Group theory in condensed matter physics

Let's first briefly review the role of group theory in quantum mechanics. We are usually interested in Lie group symmetries and discrete symmetries, the latter being more important in condensed matter physics because in this field we have to deal with lattices with point group symmetries, and many symmetries that are important for topological states of matter are associated with discrete symmetries like parity symmetry and a special symmetry for fermions named the **fermion-parity symmetry**, which exists in all fermionic systems and arises from the fact that each term in the Hamiltonian always contains even fermionic operators.

So we will just work with discrete groups hereafter. Actually we have the continuous spin rotational symmetry, but since spin-orbital coupling exists in all realistic materials, operations on the spin degrees of freedom are just a part of *doubled* space groups.

A **linear representation** is a group homomorphism from a symmetry group G to $\text{GL}(\mathcal{H})$, where $\mathcal{H}$ is the Hilbert space. Since the wave function of the system can differ a phase factor after a symmetric operation, we can also have **projective representation**. Representation theory gives very generic results for studying symmetries.

Let $\varphi(\cdot)$ be the mapping from G to $\text{GL}(\mathcal{H})$. If φ is a linear representation, then it's easy to see

$$[H, \varphi(g)] = 0, \tag{1}$$

for any group element g. We often say that $\varphi(g)$'s *label* the energy eigenstates. For Abelian symmetric group G, the labels of $|n\rangle$ are simply given by $\varphi(g_i)|n\rangle$, where $\{g_i\}$ are generators of G. If G is non-Abelian, we need to work with its irreducible representations, and energy eigenstates are classified into several irreducible representations of G, and group elements turn one state into another state in the same irreducible representation. The degeneracy of energy eigenstates is always the dimension of *one* representation. Since a reducible representation can always be split into two irreducible representations by a perturbation, from then on we only investigate energy degeneracy protected by irreducible representations.

2 Group extension and group cohomology

2.1 Group extension

Consider the following short exact sequence

$$1 \to N \xrightarrow{f} G \xrightarrow{\pi} Q \to 1. \tag{2}$$

The definition of exact sequence means

- f is injective, since $\ker f = \text{im}(\text{the monomorphism } 1 \to N) = 1$.

- π is surjective, since $\text{im}\,\pi = \ker(\text{the monomorphism } Q \to 1) = Q$.

- $Q \simeq G/\text{im}\,f$, because $G/\ker\pi = \text{im}\,\pi$, and by definition we have $\ker\pi = \text{im}\,f$, and $\text{im}\,\pi = Q$ (from last line). Note that since f is injective, $\text{im}\,f$ is a perfect copy of N, and can be seen as an inclusion map from N into G.

G is defined said to be an **extension** of Q over N.

We consider the case where N is Abelian. What we want to do is to find and classify all group extensions – under the assumption that N is Abelian, we are actually working on *central extensions*. Two group extensions are said to be **equivalent** if and only if the following diagram

$$1 \longrightarrow N \begin{array}{c} \nearrow \\ \searrow \end{array} \begin{array}{c} G \\ \uparrow \\ G' \end{array} \begin{array}{c} \searrow \\ \nearrow \end{array} Q \longrightarrow 1 \tag{3}$$

commutes, and we need to find equivalent classes of this equivalence relation.

2.2   Direct product and semidirect product

The simplest kind of group extension is just direct product: we define G to be

$$G = N \otimes Q, \tag{4}$$

and the multiplication operation is defined as

$$(a, g) \circ (b, h) := (a + b, gh). \tag{5}$$

We also have **semidirect product** or **split extension** $N \rtimes Q$, the multiplication rule of which is defined as

$$(a, g) \circ (b, h) := (a + gbg^{-1}, gh). \tag{6}$$

We also say G **splits** over N. Note that the notation gbg^{-1} is kind of ambiguous, because up to now we haven't introduced any multiplication relation between N and Q. A more accurate notation is to introduce a group homomorphism $\varphi : Q \to \mathrm{Aut}(N)$ and interpret $\varphi(g)(a)$ as $\tilde{g}a\tilde{g}^{-1}$, where $\pi(\tilde{g}) = g$. According to the definition, π is surjective and not injective, because after group extension, the same group element g in Q is "split" into several copies in G, and we use $\tilde{g}$ to denote a certain "copy" of g. (6) is therefore corrected into

$$(a, g) \circ (b, h) := (a + \tilde{g}b\tilde{g}^{-1}, gh). \tag{7}$$

We need to check whether (5) and (7) can really make G a group, i.e. we need to check whether the associative law holds for $\{(a, g)\}$. For direct product, this is obviously true. For semidirect product, we have

$$((a, g)(b, h))(c, i) = (a + \tilde{g}b\tilde{g}^{-1}, gh)(c, i)$$
$$= (a + \tilde{g}b\tilde{g}^{-1} + (\widetilde{gh})c(\widetilde{gh})^{-1}, ghi),$$

and

$$(a, g)((b, h)(c, i)) = (a, g)(b + \tilde{h}c\tilde{h}^{-1}, hi)$$
$$= (a + \tilde{g}(b + \tilde{h}c\tilde{h}^{-1})\tilde{g}^{-1}, ghi).$$

Usually, we define multiplication rules under the definition of (a, h)-pairs as is in (10), i.e. $\tilde{g} = s(g)$ and doesn't depend on a, b, and under this assumption, we have (12). So we have

$$\tilde{g}\tilde{h}c\tilde{h}^{-1}\tilde{g}^{-1} = \widetilde{gh}c\widetilde{gh}^{-1},$$

because

$$\widetilde{gh}^{-1}\tilde{g}\tilde{h}c\tilde{h}^{-1}\tilde{g}^{-1}\widetilde{gh}$$
$$= \underbrace{\widetilde{gh}^{-1}\tilde{g}\tilde{h}}_{\in \mathrm{im}\, f} + c + \underbrace{(\widetilde{gh}^{-1}\tilde{g}\tilde{h})^{-1}}_{\in \mathrm{im}\, f}$$
$$= c.$$

and therefore (7) is always self-consistent.

The motivation of semidirect product is to imitate *inner* semidirect product. An abstract definition of inner semidirect product can be found this Wikipedia page. In short, if G has a subgroup H and a normal subgroup N with no nontrivial intersection with Q, and $G = NQ$,

then we say G is the **inner semidirect product** of N and Q. (7), on the other hand, is **outer semidirect product**, and after we construct G according to it, we will find G is the inner semidirect product of $N \times e_Q$ and $0_N \times Q$.

Similarly, we have inner direct product. But it's often the case that we can only guarantee that N is normal and there is nontrivial multiplication relation between N and Q. In this case, G simply can't be written as the (outer) direct product of N and Q, and if we still want to *factor* G into something like $N \times Q$, inner *semidirect* product will be handy. This explains the motivation to introduce (7). (We can define $N \times Q$, but the result doesn't have the same structure with G.)

2.3 Generic group extensions and their equivalence relations

Now we want to investigate a generic central extension. The multiplication rule is

$$(a, g) \circ (b, h) \coloneqq (a + \tilde{g} b \tilde{g}^{-1} + \omega_2(g, h), gh), \tag{8}$$

where

$$\omega_2 : Q \times Q \to N. \tag{9}$$

Here we assume that ω_2 is only dependent on g and h and doesn't include a and b, because of the argument below. Since π is surjective, we can find a map s from Q to G such that $\pi \circ s = \mathrm{id}_Q$. Note that s is not necessarily a homomorphism, or otherwise (2) is split. Usually we define

$$(a, g) = f(a) s(g) \tag{10}$$

to derive multiplication rules. A little calculation gives

$$\begin{aligned}
(a, g) \circ (b, h) &= f(a) s(g) f(b) s(h) \\
&= f(a) s(g) f(b) s(g)^{-1} s(g) s(h) s(gh)^{-1} s(gh).
\end{aligned} \tag{11}$$

Note that since π is a homomorphism, we have

$$\begin{aligned}
\pi(s(g) s(h) s(gh)^{-1}) &= \pi(s(g)) \pi(s(h)) \pi(s(gh))^{-1} \\
&= gh(gh)^{-1} = e,
\end{aligned}$$

and the derivation also works for $s(gh)^{-1} s(g) s(h)$, so we have

$$s(gh)^{-1} s(g) s(h), s(g) s(h) s(gh)^{-1} \in \ker \pi = \operatorname{im} i, \tag{12}$$

So (11) is now

$$(a, g) \circ (b, h) = (f(a) + s(g) f(b) s(g)^{-1} + \underbrace{s(g) s(h) s(gh)^{-1}}_{\coloneqq \omega_2(g,h)}) s(gh),$$

and we get (8).

The next step is to check the constraint on ω_2 to ensure that G is really a group. From

$$((a, g) \circ (b, h)) \circ (c, i) = (a, g) \circ ((b, h) \circ (c, i)),$$

we have

$$\omega_2(g, h) + \omega_2(gh, i) = \underbrace{\tilde{g} \omega_2(h, i) \tilde{g}^{-1}}_{g \cdot \omega_2(h,i)} + \omega_2(g, hi). \tag{13}$$

This constraint on ω_2 seems strange, but actually it's a part of a larger structure: **group cohomology**.

2.4 Group cohomology

A cohomology structure can be illustrated as

$$\cdots \to C^{n-1} \xrightarrow{\mathrm{d}_{n-1}} C^n \xrightarrow{\mathrm{d}_n} C^{n+1} \to \cdots, \tag{14}$$

where

$$\mathrm{d}_{n+1} \circ \mathrm{d}_n =: \mathrm{d}^2 = 0, \tag{15}$$

and

$$\mathrm{im}\,\mathrm{d}_{n-1} = \ker \mathrm{d}_n. \tag{16}$$

An element $\omega \in C^n$ is an n-**cochain**. An n-cochain ω is said to be an n-**cocycle** if and only if $\mathrm{d}\omega = 0$, the set of which is denoted as

$$Z^n = \ker \mathrm{d}_n. \tag{17}$$

and an n-cochain ω is said to be an n-**coboundary** if and only if $\omega = \mathrm{d}\mu$, the set of which is denoted as

$$B^n = \mathrm{im}\,\mathrm{d}_{n-1}. \tag{18}$$

Of course, n-coboundaries are all n-cocycles, but not inverse. A natural equivalence relation between n-cocycles is that

$$\omega \sim \omega' \quad \text{iff} \quad \omega - \omega' \in B^n, \tag{19}$$

and the set of equivalence classes is

$$H^n = Z^n / B^n. \tag{20}$$

If (14) is exact, then H^n's are trivial. Cohomology is a tool to measure how *inexact* (14) is.

For groups, one possible way to obtain cohomology is to define

$$C^n(G, N) := C^n \to N, \tag{21}$$

and

$$(\mathrm{d}_n\omega)(g_1, \ldots, g_{n+1}) := g_1 \cdot \omega(g_2, \ldots, g_{n+1}) + \sum_{i=1}^{n}(-1)^i \omega(g_1, \ldots, g_i g_{i+1}, \ldots, g_{n+1})$$
$$- (-1)^n \omega(g_1, \ldots, g_n). \tag{22}$$

We also assume that d and $g\cdot$ commute. Now we verify the $\mathrm{d}^2 = 0$ condition. We have

$$\mathrm{d}_{n+1}(\{g_i\}_{i=1}^{n+1} \mapsto g_1 \cdot \omega(g_2, \ldots, g_{n+1}))(g_1', \ldots, g_{n+2}')$$
$$= g_1' g_2' \cdot \omega(g_3', \ldots, g_{n+2}') + \sum_{i=1}^{n+1}(-1)^i g_1' \cdot \omega(g_2', \ldots, g_i' g_{i+1}', \ldots, g_{n+2}') - (-1)^{n+1} g_1' \cdot \omega(g_2', \ldots, g_{n+1}'),$$

$$\mathrm{d}_{n+1}(\{g_i\}_{i=1}^{n+1} \mapsto \omega(g_1, \ldots, g_n)) =$$

$$\cdots \to C^{n-1}(G, N) \xrightarrow{\mathrm{d}^{n-1}} C^n(G, N) \xrightarrow{\mathrm{d}^n} C^{n+1}(G, N) \to \cdots, \tag{23}$$

Specifically, we have

$$\mathrm{d}\omega\,(g_1, g_2, g_3) = g_1 \cdot \omega(g_2, g_3) - \omega(g_1 g_2, g_3) + \omega(g_1, g_2 g_3) - \omega(g_2, g_3), \tag{24}$$

and this means the self-consistent constraint (13) on ω_2 appearing in (8) is just equivalent to

$$\mathrm{d}\omega_2 = 0 \quad \text{or in other words} \quad \omega_2 \in Z^2(G, N). \tag{25}$$

The fact ω_2 in (8) being a 2-cocycle hints us that classification of possible ω_2's can also be done in terms of group cohomology. We need to check the condition whether ω_2 is equivalent to ω_2'.

3 Space groups

In this section we are not going to show that there are 230 space groups in $\mathbb{R}^3$. Actually we usually call 2D space groups as **wallpaper groups**. A group element of a space group is in the form of the following affine transformation

$$(R|\boldsymbol{t}) : \boldsymbol{v} \mapsto R\boldsymbol{v} + \boldsymbol{t}, \tag{26}$$

or in the form of

$$(R|\boldsymbol{t}) : \tilde{\boldsymbol{v}} := \begin{pmatrix} \boldsymbol{v} \\ 1 \end{pmatrix} \mapsto \underbrace{\begin{pmatrix} R & \boldsymbol{t} \\ 0 & 1 \end{pmatrix}}_{:=\tilde{R}} \tilde{\boldsymbol{v}}, \tag{27}$$

which is the preferred form of space group operation in numerical calculations.

Detailed discussion on the structure of space groups can be found in Section. 2.2.5 in this note. Here we list some of the elements. First we discuss point groups. We have C_n axises, the generator of which is labeled as n: we have 1, 2, 3, 4, 6 axises, the first being the identity. We also have rotation-reflection axises $\bar{1}, \bar{2}, \bar{3}, \bar{4}, \bar{6}$, the first being the inversion operation and the second being the mirror reflection. $\bar{3}$ is not an independent generator because we have

$$(\bar{3})^3 = \bar{1}, \quad \bar{3}\bar{1} = 3.$$

Similarly, $\bar{6}$ is also not an independent generator.

There are also **nonsymmorphic** operations, which involve fraction translation. There are two types of nonsymmorphic generators: **screw axis** $(c_n|n\boldsymbol{R}/m)$, where $m = 1, 2, 3, \ldots$, and **glide plane** $(\sigma|\boldsymbol{R}/2)$.

We can find the "deep" reason of the emergence of nonsymmorphic operations . The point group of a space group G is $K = G/\mathbb{T}$, where $\mathbb{T}$ is the translation group. Note that if G is nonsymmorphic, K is *not* a subgroup of G. For symmorphic space groups, G is *semidirect* product of K and $\mathbb{T}$. We have

$$G = \mathbb{T} \rtimes K. \tag{28}$$

4 Wave vector star and little group

We define the **little group** of G to be the subgroup of G where every group element keeps the wave vector invariant, i.e.

$$LG_{\boldsymbol{k}} = \{g \in S | g\boldsymbol{k} \simeq \boldsymbol{k}\}, \tag{29}$$

where $\simeq$ means two wave vectors being equivalent, i.e. differ with a $\boldsymbol{R}_m$. We define $\boldsymbol{k}^*$ to be the set of wave vectors that can be obtained by acting G on $\boldsymbol{k}$, and we have

$$|\boldsymbol{k}^*| = \frac{|G|}{|LG|}. \tag{30}$$

Since T is a normal subgroup of $LG_{\boldsymbol{k}}$, we define the **little cogroup**

$$PG_{\boldsymbol{k}} = \{g \in G/\mathbb{T} | g\boldsymbol{k} \simeq \boldsymbol{k}\} = LG_{\boldsymbol{k}}/\mathbb{T}. \tag{31}$$

This gives a short exact sequence:

$$1 \to \mathbb{T} \to LG_{\boldsymbol{k}} \to PG_{\boldsymbol{k}} \to 1. \tag{32}$$

Now if we know all irreducible representations of $LG_{\boldsymbol{k}}$, then we can easily construct Representations of space groups can be found in Bilbao Server.