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Group Theory Essentials

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1 Introduction

These notes are intended to provide the bare essentials needed for discussing problems in introductory quantum mechanics using group-theoretical language, which often helps to clarify what is going on in otherwise mysterious processes, such as angular momentum addition. The serious student should find a more serious treatment. There are many books and various internet sources which provide helpful material on groups. Among the former:

M. Hamermesh, *Group Theory and its Application to Physical Problems* (Addison-Wesley, 1962).

S. K. Kim, *Group Theoretical Methods* (Cambridge, 1999)

M. Tinkham, *Group Theory and Quantum Mechanics* (McGraw-Hill, 1964)

W-K. Tung, *Group Theory in Physics* (World Scientific, 1985)

2 Definitions

$\odot$ A group is a set G of elements which will be denoted by lower case letters: $g, h, \ldots$ with the following features:

(i) For every pair of elements g and h in G the *product* gh is an element in G. Sometimes one writes the product with a dot: $g \cdot h$. Terminology: gh is h multiplied on the left by g, which is the same things as g multiplied on the right by h.

(ii) Multiplication is *associative*: $f(gh) = (fg)h$, where $f(gh)$ means take the product of g and h first, and then multiply on the left by f.

(iii) There is a special unique element of G, the *identity*, here denoted by e, such that

$$eg = ge = g \text{ for every } g \in G \tag{1}$$

(iv) For every $g \in G$ there is another element (which could be g itself), commonly denoted by g^{-1}, such that

$$g^{-1}g = g^{-1}g = e. \tag{2}$$

• A group in which the multiplication is commutative, which is to say $gh = hg$ for every pair of elements in G, is known as a *commutative* or *abelian* (or *Abelian*) group. If there are cases in which $gh \neq hg$, the group is *noncommutative* or *nonabelian*.

⊙ The number of elements $|G|$ in the set G is the *order* of the group.

∘ The easiest groups to think about are *finite* groups, but physicists also use infinite groups, both countable and uncountable.

⊙ A *subgroup* H of G is a subset of elements to which the same multiplication rules apply, and which forms a group by itself. Of necessity H will contain the identity e of G, and if it contains g it must contain g^{-1}. This definition allows e by itself to be a subgroup, and G to be a subgroup of G. If you want to exclude these cases, ask for a *proper* subgroup of G.

⊙ Examples: Integers under addition with $n \cdot m$ defined to be $n + m$ is an abelian group. As are: real numbers under addition; real numbers excluding 0 under multiplication.

⋆ Exercise. For each of the groups just mentioned, what is the identity e? Give a reason why 0 was omitted from the real numbers when forming a group using (ordinary) multiplication.

⋆ Exercise. Construct a proper subgroup of the integers under addition.

⋆ Exercise. The integers under multiplication do not form a group, even if one excludes 0. What goes wrong? Fix it by making G a larger set of numbers that include the integers, but keep it as small as possible.

• Example: The 2×2 Pauli matrices

$$\sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3}$$

along with their products and products of products, etc., are an example of a nonabelian group, which we call the *Pauli group*.

⋆ Exercise. Find all the elements of the Pauli group. What is its order?

⋆ Exercise. Construct a proper subgroup of the Pauli group.

⋆ Exercise. Must a proper subgroup of an abelian group be abelian? Must a proper subgroup of a nonabelian group be nonabelian?

⊙ Two group elements f and g are said to be *conjugate*, $f \sim g$ provided there is an element $h \in G$ such that

$$f = hgh^{-1}. \tag{4}$$

• It is clear that $f \sim g$ implies $g \sim f$—multiply both sides of (4) by h^{-1} on the left and h on the right—and that $g \sim g$ (let $h = e$) for every g. Thus *conjugacy* is an equivalence relation, and the set G can be written as a union of nonoverlapping *conjugacy classes*, often referred to simply as *classes*. In each class every element is conjugate to every other element.

⋆ Exercise. Show that e is always in a conjugacy class by itself, and that in an abelian group every element is in its own conjugacy class.

⊙ Two groups G and H are said to be *isomorphic* if there is a one-to-one map or *bijection* from G to H which preserves the group operations. Let $\phi : G \to H$ be the bijection. We require that

$$\phi(e) = \text{ identity on } H, \quad \phi(fg) = \phi(f)\phi(g), \quad \phi(g^{-1}) = \phi(g)^{-1}. \tag{5}$$

• One refers to such a ϕ, or its inverse map $\phi^{-1} : H \to G$, which satisfies a set of properties analogous to those in (5), as an *isomorphism*.

◦ Two groups which are isomorphic are in some sense "the same": once you understand one of them you understand the other. So one sometimes uses the same name for both.

⊙ A *homomorphism* from the group G to the group H is a map ϕ that satisfies the properties in (5) but is not required to be one-to-one, so in general the inverse will not exist. One says that H and G are *homomorphic*

◦ It is useful to define "homomorphisms" in such a way as to include isomorphisms as a special case.

3 Symmetry Group D_3 of the Equilateral Triangle

⊙ The dihedral group $D_3 = \{e, a, b, c, r, s\}$ is of order 6. Geometrically it represents the symmetries of an equilateral triangle; see Fig. 1 below. It is isomorphic to the group S_3 of all permutations of three objects.

• Multiplication table. Here the product fg of two group elements is the element that occurs at the intersection of row f and column g; e.g. $br = c$.

	e	a	b	c	r	s
e	e	a	b	c	r	s
a	a	e	r	s	b	c
b	b	s	e	r	c	a
c	c	r	s	e	a	b
r	r	c	a	b	s	e
s	s	b	c	a	e	r

◦ The table is not symmetrical across the main diagonal (upon interchanging rows and columns). Thus D_3 is not abelian.

◦ From the table itself it is not immediately obvious that the multiplication is associative. (It is, but checking it takes some work, and the task is easier if one uses generators; see below.)

⊙ In geometrical terms, the group D_3 is the symmetry group of an equilateral triangle, i.e., the collection of transformations that maps the triangle onto itself. For ease of discussion we place the triangle in the x, y plane as shown here, with its vertices labeled $1, 2, 3$. Then a, b, c are reflections about the dashed lines (in three dimensions 180° rotations about these lines), while r and s are 120° clockwise and counterclockwise rotations.

⊙ The reflection a interchanges vertices 2 and 3 while leaving 1 fixed, whereas r maps 1 to 2 to 3.

• Thus we can associate these operations with with permutations of the integers $\{1, 2, 3\}$.

$$e = (), \;\; a = (23), \;\; b = (13), \;\; c = (12), \;\; r = (123), \;\; s = (132). \tag{6}$$

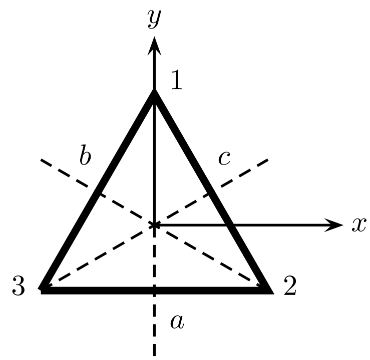

Figure 1: Equilateral triangle and its symmetries

Here () is the identity permutation. In fact these are all the 6 permutations possible on $\{1, 2, 3\}$, so D_3 is isomorphic to the group S_3 of permutations of three objects.

⊙ Rather than constructing a group multiplication table it is often easier to construct group elements using a smaller number of *generators* of the group.

• For D_3 one can use two generators r and a, and write the other elements in terms of them:

$$e = r^3 = a^2; \quad s = r^2; \quad b = ar; \quad c = ar^2. \tag{7}$$

◦ The choice of generators is not unique. One could just as well use s and c.

• Given two generators one can potentially use them to generate an enormous group using products such as $r^m a^n r^p a^q \cdots$. However, in the present case all of these possible products can be shown to give rise to only six distinct elements. This is done by using what are called *relations*. To be systematic, relations are supposed to be written in the form product-of-generators-to-some-powers $= e$. For the case at hand one needs three relations; here is an appropriate set (the choice is not unique):

$$a^2 = e; \quad r^3 = e; \quad arar = e \tag{8}$$

⋆ Exercise. Use the relations in (8) to obtain $ra = ar^2$, $r^2 a = ar$. Then explain how to put any product $r^m a^n r^p a^q \cdots$, assuming it is of finite length, into the form $a^s r^t$, where $s = 0$ or 1 and $t = 0$, 1, or 2. (We use the convention that any group element raised to the power 0 is e).

⊙ Rotations about the origin and reflections in lines through the origin of the x, y plane can be represented by matrices. Thus a counterclockwise rotation by an angle θ will move a point (x, y) to a new point (x', y'), where

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}. \tag{9}$$

• Thinking of the elements of D_3 as mapping the plane in the manner shown in Fig. 1, we can associate them with 2×2 matrices as follows, where I corresponds to the identity e, A to a, etc.

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \; A = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \; B = \frac{1}{2}\begin{pmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}, \; C = \frac{1}{2}\begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix},$$
$$R = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}, \; S = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} \tag{10}$$

• The group operation then corresponds to, or can be represented by, matrix multiplication. Thus

$$AR = \frac{1}{2}\begin{pmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix} = B \tag{11}$$

in agreement with $ar = b$ from the group multiplication table.

⊙ Subgroups of D_3. There are four proper subgroups:

$$F_a = \{e, a\} = \langle a\rangle,\ \ F_b = \{e, b\} = \langle b\rangle,\ \ F_c = \{e, c\} = \langle c\rangle,\ \ F_r = \{e, r, s\} = \langle r\rangle, \tag{12}$$

• Here $\langle a\rangle$ means the subgroup *generated by* a. It consists of a, $a^2, \ldots a^p = e$, where p is the *order* of a. In a finite group the order of a is necessarily finite. But in an infinite group the order of a may be infinite, in which case one should also include $e = a^0, a^{-1}, a^{-2}, \ldots$ along with positive powers of a in $\langle a\rangle$.

4 Representations

4.1 Basic definitions

⊙ For our purposes a *representation* of a group G is a collection $\mathcal{R}$ of linear operators on a complex vector space, together with a homomorphism ϕ from G to R in which group multiplication is mapped to the product of operators, and group inverse to the inverse of the operator. Hence ϕ maps the identity e of G to the identity operator I on the vector space. As we denote operators by capital letters, let us write

$$R(g) = \phi(g) \tag{13}$$

• Given a basis of a vector space, the linear operators can be represented by *matrices*, and therefore one can always think of a representation as made up of a collection of matrices. Sometimes the "operator" perspective is more useful, but often the "matrix" perspective is easier to visualize. So learn both.

∘ Example: If G is the dihedral group of Sec. 3, the collection $\mathcal{R}$ of matrices in (10) forms a representation.

⊙ If the homomorphism is an isomorphism, which is to say ϕ maps distinct elements of G to distinct operators $R(g)$ one says that the representation is *faithful*; otherwise, when the map is many-to-one, the representation is unfaithful.

• Any group G always has a representation in which every g is mapped to the identity operator I. This is called an *identity* or *trivial* representation. Do not interpret "trivial" to mean "uninteresting", or "you can ignore it."

⊙ Two representations $\mathcal{R}$ and $\mathcal{S}$ of the same group are said to be *equivalent* provided the corresponding operators are related by a similarity transformation: a linear operator T with inverse T^{-1} such that

$$S(g) = TR(g)T^{-1}. \tag{14}$$

It is important that this hold for *all* $g \in G$ using a *single* g-independent operator T.

∘ It might be that $\mathcal{R}$ and $\mathcal{S}$ are defined on two separate vector spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, in which case T in (14) has to be an invertible map from $\mathcal{H}_1$ to $\mathcal{H}_2$, with T^{-1} a map from $\mathcal{H}_2$ to $\mathcal{H}_1$. Of course the dimensions of $\mathcal{H}_1$ and $\mathcal{H}_2$ must be the same.

⊙ For most of the applications of interest to us the representation vector space $\mathcal{H}$ is a Hilbert space, and the linear maps representing the group can be chosen to be *unitary*. This simplifies the discussion somewhat. Note that the operator product of two unitaries is unitary, and the inverse of a unitary is its adjoint, so we have $R(g^{-1}) = R^\dagger(g)$.

4.2 Reducible and irreducible

⊙ A representation of a group is said to be *reducible* if all the $R(g)$ map a *proper subspace* of $\mathcal{H}$ onto itself: "proper" means neither the whole space itself, nor the trivial subspace containing just the 0 vector. A somewhat stronger notion of reducibility is that of being *completely reducible* or *fully reducible* or *decomposable* or *semisimple*. Let us use "completely reducible."

⊙ To clarify what is meant it is helpful to think about representation matrices in terms of *blocks*, as indicated schematically in

$$R(g) = \begin{pmatrix} A(g) & B(g) \\ C(g) & D(g) \end{pmatrix} \tag{15}$$

where $A(g)$ is a square $m \times m$ matrix, $D(g)$ a square $n \times n$ matrix, while $B(g)$ and $C(g)$ are rectangular (square when $n = m$) $m \times n$ and $n \times m$ matrices. Here $m > 0$ and $n > 0$ are positive integers whose sum is the dimension of the representation; i.e., $R(g)$ is an $(m+n) \times (m+n)$ matrix.

∘ The form of these matrices depends, of course, on the choice of basis. It is important that the *same* basis be used for *all* $g \in G$.

• If one can find a basis in which both $C(g) = 0$—all the matrix elements are zero, for *every* g—then the representation is $\mathcal{R}$ *reducible*. If one can choose a basis such that $B(g) = 0$ *and* $C(g) = 0$, the representation is *completely reducible*.

∘ Most of the time we will be interested in completely reducible representations. For example, representations of finite groups are always completely reducible (Hamermesh, p. 98), and Hamermesh himself (same page) uses "reducible" to mean "completely reducible." Tinkham also uses "reducible" in this sense. We will follow their example.

⊙ A representation that is not reducible is, of course, *irreducible*. Much of the practical utility of groups in physics hinges in knowing something about the irreducible representations or *irreps* of the group one is interested in.

• To begin with, two irreducible representations may be equivalent, in which case we think of them as the same irrep. So the question is: what are the *inequivalent* irreps of the group G?

⊙ Take the example of D_3, Sec. 3. It has precisely three inequivalent irreps.

• One of them is the two-dimensional irrep given in (10). That this is irreducible follows from the observation that if we could simultaneously block-diagonalize the set of 6 matrices they would all be diagonal and commute with each other, but they don't.

• One irrep is the trivial irrep: each g is mapped to 1, thought of as a 1×1 matrix.

• The remaining irrep is similarly one-dimensional, but now e, r, and s are mapped to 1, and a, b, and c are mapped to -1.

⋆ Exercise. Check that this last is a representation.

• To show that these three irreps exhaust the list for D_3 (up to equivalence, of course) is one of those things that requires a nontrivial argument, for which see the books.

⊙ The irreps of an *abelian* group are one-dimensional, since they have to commute with each other. On the other hand, a nonabelian group like D_3 has at least one irrep of dimension greater than 1.

4.3 Characters and the character table

⊙ If $R(g)$ is the matrix representing $g \in G$ in the representation $\mathcal{R}$, one defines the *character* of g in this representation by

$$\chi(g) = \mathrm{Tr}[R(g)]. \tag{16}$$

Likewise the collection of all the $\chi(g)$ for every g in G is called the *character* of the representation $\mathcal{R}$.

○ We are assuming the representation is finite-dimensional, as otherwise the trace of a matrix will (in general) not be defined.

• It is straightforward to show, using the cyclic property of the trace, that two elements g and h in the same conjugacy class have the same character.

• Similarly straightforward: two equivalent representations have the same character.

⋆ Exercise. Provide a proof of these straightforward results.

• For one-dimensional representations the character is the same as the representation matrix, and so in this sense the character (thought of as a function of g) *is* the representation.

⊙ The *character table* for a group G consists of a set of rows, one for each (inequivalent) irrep, and columns labeled by the different elements of G, such that each row gives the set of characters for that particular irrep.

• As an example, here is the character table of D_3.

D_3	e	r	s	a	b	c
$\mu = 1$	1	1	1	1	1	1
$\mu = 2$	1	1	1	−1	−1	−1
$\mu = 3$	2	−1	−1	0	0	0

The different irreps are labeled by an index μ given in the left column. There are no "standard" labels; authors use different conventions. The trivial irrep always occupies the top row.

○ Observe that the rows are mutually orthogonal and normalized in the sense that

$$|G|^{-1} \sum_{g \in G} \chi_\mu^*(g) \chi_\nu(g) = \delta_{\mu\nu}. \tag{17}$$

This is a very general and useful result which holds for any finite group; $|G|$ is the order of the group.

⊙ In books the character table of D_3 given in a more compact form

D_3	e	$\{r, s\}$	$\{a, b, c\}$
$\mu = 1$	1	1	1
$\mu = 2$	1	1	−1
$\mu = 3$	2	−1	0

Here one uses the fact that the character is the same for elements in the same conjugacy class, in order to save space. The rows are still orthogonal (and have the same normalization) provided one remembers to insert a factor equal to the number of elements in the conjugacy class when working out an expression like (17). The conjugacy classes are labeled in various different ways by different authors.

• This compact table is a square matrix. A general result which holds for all finite groups is that the number of (inequivalent) irreps is the same as the number of conjugacy classes.

⊙ Given a reducible representation of G, there will be a basis in which the matrices have block-diagonal form. Either the blocks are irreps, or else by further adjusting the basis one can turn each reducible block into smaller blocks, until every block is an irrep. The different blocks need not correspond to inequivalent irreps; a particular irrep may occur several times.

• The trace of the matrix $R(g)$ does not depend upon the basis, and if one thinks of $R(g)$ in block diagonal form corresponding to the different irreps, it is evident that the character $\chi(g) = \mathrm{Tr}[R(g)]$ is the sum of the characters of all the irreps that are present.

• The preceding observation makes it possible to determine which irreps are present, and how often each (inequivalent) irrep is present, in some reducible representation $\mathcal{R}$ without trying to simultaneously block diagonalize each of its matrices. Instead, calculate the character of $\mathcal{R}$: one (in general complex) number for every g in G. This character must then be the sum of some of the rows in the character table, each row multiplied by the number of times that particular irrep occurs in $\mathcal{R}$:

$$\chi(g) = \sum_{\mu} \nu_\mu \chi_\mu(g) \tag{18}$$

for some collection of nonnegative integers $\{\nu_\mu\}$.

◦ Suppose, for example, you are handed a messy collection of 4×4 matrices which form a representation of D_3. Clearly this cannot be an irreducible representation. So what is likely to be present? Form the character of each element. Let us suppose that $\chi(r) = \chi(s) = 0$, $\chi(a) = -2$. Of course $\chi(e) = 4$, since e is always represented by the identity operator. A glance at the character table would suggest that what I have called $\mu = 2$ is present twice, and $\mu = 3$ is present once; the characters in the table then add up correctly. But is guessing the answer an honest procedure? Yes, because the rows in the character table are orthogonal, and so they represent linearly independent functions of g, and so the answer will be unique.

• For those who prefer not to guess, or if the representation is really big and complicated: Multiply both sides of (18) by $\chi_\lambda^*(g)$, sum over g, and use (17) to extract the value of ν_λ.

4.4 Classifying functions by irreps

⊙ Everyone knows that any function $f(x)$ of the real variable x can be written as the sum of an *even* function $f_e(x)$ and an *odd* function $f_0(x)$

$$f(x) = f_e(x) + f_o(x), \tag{19}$$

where

$$f_e(x) = \tfrac{1}{2}[f(x) + \Pi f(x)], \quad f_o(x) = \tfrac{1}{2}[f(x) - \Pi f(x)]; \text{ where } (\Pi f)(x) = f(-x). \tag{20}$$

• This is an example of a very general and useful procedure. Given a group G and a representation of G on a vector space $\mathcal{V}$, it is possible to write any vector in the space as a sum of vectors associated with the different irreps of the group. In the case at hand the vector space $\mathcal{V}$ is the set of all functions $f(x)$. (One could restrict it to square integrable functions). The group consists of two elements: $\{e, p\}$, where $p^2 = e$, and we represent it on $\mathcal{V}$ by $R(e) = I$ and $R(p) = \Pi$. There are two irreps: the trivial one and the one with $e \to 1$, $p \to -1$. The even and functions correspond to these two irreps in the sense that

$$I f_e = f_e, \;\; \Pi f_e = f_e; \quad I f_o = f_o, \;\; \Pi f_o = -f_o \tag{21}$$

• It is also worth noting that the even and odd parts can be "extracted" from a general $f(x)$ by using projection operators (square of the operator is equal to itself); one can rewrite (20) as

$$f_e = P_e f, \;\; f_o = P_o f; \quad P_e = \tfrac{1}{2}(I + \Pi), \;\; P_o = \tfrac{1}{2}(I - \Pi) \tag{22}$$

⊙ These ideas can be extended to more general groups, and as one might guess, the projection operators can be constructed from the operators $R(g)$ that represent the group along with the characters in its character table.

5 Symmetry Group of the Hamiltonian

⊙ Groups and group representations have many uses in quantum mechanics. One of the simplest and most straightforward is the *symmetry group of the Hamiltonian*, by which we mean the following. The Hamiltonian is a Hermitian operator H on some Hilbert space $\mathcal{H}$. We say that its symmetry group $\mathcal{G}$ consists of all *unitary* operators U which *commute* with H, or they leave H *invariant*, i.e.,

$$UH = HU \text{ or } H = UHU^\dagger. \tag{23}$$

• It is obvious that $\mathcal{G}$ contains the identity, and $U \in \mathcal{G}$ if and only if $U^{-1} = U^\dagger$ is in $\mathcal{G}$. Less obvious, but pretty straightforward: if both U and V are in $\mathcal{G}$, then both UV and VU, which need not be the same, are in $\mathcal{G}$.

⋆ Exercise. Prove the less obvious point.

∘ Why limit $\mathcal{G}$ to *unitary* operators? Because this is usually sufficient, although there are cases in which one also wants to include antiunitary operators (time reversal is the infamous example) in $\mathcal{G}$. Let us stick with simplicity....

• Example. Particle in one dimension. If $V(x)$ is constant, H is left unchanged by all translations and reflections. If $V(x)$is not constant, but $V(x) = V(-x)$, then H is left unchanged by a reflection Π through the origin, so $\mathcal{G} = \{I, \Pi\}$.

⊙ Let us suppose that we have a situation where the energy eigenvalues are discrete, so we can write

$$H = \sum_j \epsilon_j P_j; \quad \epsilon_j \neq \epsilon_k \text{ for } j \neq k. \tag{24}$$

I.e., P_j is the projector onto the j'th *energy eigenspace*, the space spanned by all eigenvectors with eigenvalue ϵ_j.

⊙ Theorem. The subspace $\mathcal{S}_j$ of $\mathcal{H}$ onto which P_j projects, the energy eigenspace associated with ϵ_j, is a representation of $\mathcal{G}$.

∘ Proof. We need to show that for $U \in \mathcal{G}$ and $|\psi\rangle$ in $\mathcal{S}_j$, $U|\psi\rangle$ is also in $\mathcal{S}_j$; that is, the operators in $\mathcal{G}$ map $\mathcal{S}_j$ to itself. Here is the demonstration:

$$H(U|\psi\rangle) = UH|\psi\rangle = U(\epsilon_j|\psi\rangle) = \epsilon_j(U|\psi\rangle). \tag{25}$$

So $U|\psi\rangle$ is an eigenstate of H with eigenvalue ϵ_j, and thus belongs to $\mathcal{S}_j$.

⊙ Folk theorem. The energy eigenspace $\mathcal{S}_j$ associated with ϵ_j is an *irreducible* representation of $\mathcal{G}$.

• The folk theorem is not true in general, but works in many cases, and this allows a useful *classification* of energy eigenspaces using irreducible representations of the symmetry group of the Hamiltonian.

∘ Example. Particle in one dimension with $V(x) = V(-x)$, so $\mathcal{G} = \{I, \Pi\}$. The eigenspaces correspond to even and odd functions. Hence one expects the eigenvalues of H to be nondegenerate (all irreps are one dimensional), and each eigenfunction to be either even or odd. For some cases where $V(x) = V(-x)$ (harmonic oscillator, particle in a rectangular well) one can work out the answer explicitly and show that the energy eigenstates are nondegenerate, and even or odd.

• When the folk theorem fails, i.e., the energy eigenspace is a reducible representation, this is interesting, because it means that something is special, or maybe the actual symmetry group of $\mathcal{H}$ is bigger than what one first thought it was.

• Various irreps of the rotation group play a central role in classifying energy eigenstates in atomic and nuclear physics. For example, the symbol ${}^2P_{3/2}$ used for an energy level in the sodium atom contains three parts, the superscript, the P, and the subscript, and all three refer to irreducible representations of the rotation group.

6 Rotations

⊙ Nonsingular square $n \times n$ matrices can be used to represent groups, but they themselves also form a group $GL(n)$, the *general linear group*. One often distinguishes different types of GL depending upon whether one is using real or complex numbers or some other field.

• In discussions of rotations three matrix groups play a central role: The group of *real orthogonal* 3×3 matrices $O(3)$ represent rotations and reflections, while the subgroup $SO(3)$ of real orthogonal matrices with determinant 1 correspond to *proper rotations* (reflections not allowed). The group $SU(2)$ of 2×2 unitary matrices with determinant 1 is closely connected with $SO(3)$

• To understand what is going on it helps to begin with $SO(2)$ and $O(2)$, which are easier to analyze than $SO(3)$ and $O(3)$ (and are isomorphic to certain subgroups of the latter).

6.1 Group $SO(2)$

⊙ The group $SO(2)$ consists of the matrices

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \tag{26}$$

for $-\pi < \theta \le \pi$.

∘ One can think of these as rotations about the z axis by an angle of θ, in which case the 2×2 matrices in (26) are maps of the x, y plane onto itself

• This is an example of a *continuous* group which has an uncountably infinite collection of elements labeled by a *single* real parameter θ. Group multiplication then corresponds to the map which carries the pair θ, θ' to $\theta + \theta'$ modulo 2π, whereas the inverse corresponds to $\theta \to -\theta$.

⊙ Since $SO(2)$ is abelian, we expect its irreps to be one-dimensional, and therefore the matrices in (26) form a reducible representation.

⋆ Exercise. Find a 2×2 unitary U, independent of θ, such that the matrices $UR(\theta)U^\dagger$ are diagonal.

• The irreps of $SO(2)$ are, in fact—remember that the character of a 1-dimensional representation *is* the representation—

$$\chi_n(\theta) = e^{-in\theta}, \tag{27}$$

where n is any integer, and different n correspond to different irreps. Observe that we have an infinite number of representations, which is not too surprising since we have an infinite number of conjugacy classes. (Since this group is abelian each element is in a class by itself.)

⊙ The theory of Fourier series tells us that a periodic, complex-valued function

$$f(\bar\theta) = f(\bar\theta + 2\pi) \tag{28}$$

(at least it it is not too ill-behaved) can be expanded in a Fourier series:

$$f(\bar\theta) = \sum_{n=-\infty}^{\infty} c_n e^{in\bar\theta}, \tag{29}$$

which is for this situation the counterpart of (19): expanding a function in terms of irreps of a particular group.

• To work out the connection first define a collection of linear operators $\{U(\theta\}$, one for each $R(\theta)$ in the group, acting on the space of periodic functions for each θ (labeling the group elements $R(\theta)$) on the space of periodic functions (28):

$$U(\theta)f(\bar{\theta}) = f(\bar{\theta} - \theta). \tag{30}$$

⋆ Exercise. Find functions $f_n(\bar{\theta})$ such that

$$U(\theta)f_n(\bar{\theta}) = \chi_n(\theta)f_n(\bar{\theta}) \tag{31}$$

and explain in what sense these are analogous to the even and odd $f_e(x)$ and $f_o(x)$ of Sec. 4.4.

⋆ Exercise. Can you work out the projector P_n, analogous to the P_e and P_o in (22), which in the present circumstance extracts the part of $f(\bar{\theta})$ corresponding to irrep n? [Hint: It is a linear operator acting on the function space of periodic functions of $\bar{\theta}$, and it involves an integral.]

6.2 Group $O(2)$

⨀ The group $O(2)$, the real orthogonal 2×2 matrices, includes the matrices $R(\theta)$ defined in (26), and in addition a collection of matrices

$$S(\phi) = \begin{pmatrix} \cos\phi & \sin\phi \\ \sin\phi & -\cos\phi \end{pmatrix}, \tag{32}$$

where ϕ lies in the range $-\pi < \phi \leq \pi$.

• Note that each element of $O(2)$ is either an $R(\theta)$ matrix *or* an $S(\phi)$ matrix. The identity is $R(0)$. Think of θ and ϕ as lying on two separate circles which together form a disconnected one-dimensional manifold.

⋆ Exercise. Work out explicitly, using products of 2×2 matrices, the products $R(\theta)R(\theta')$, $R(\theta)S(\phi)$, $S(\phi)R(\theta)$, $S(\phi)S(\phi')$, $R^{-1}(\theta)$, and $S^{-1}(\phi)$. In each case the result will be either an R matrix for some angle or an S matrix for some angle.

⋆ Exercise. The reflection $S(\phi)$ must be a reflection about a line in the x, y plane. What is this line? (The angle ϕ is chosen so that $S(0)$ is a reflection in the x axis.)

⋆ Exercise. What are the conjugacy classes of O(2)? [Hint: work out $GR(\theta)G^{-1}$ and $GS(\phi)G^{-1}$ for the different G that occur in $O(2)$.]

⨀ The group $O(2)$ is not abelian, so one expects that it must have some two-dimensional irreps.

⋆ Exercise. What are the irreps of $O(2)$? Write them down as matrices and provide some explanation. Your result should be plausible; you are not expected to prove things. [Hint. Most of the irreps are two dimensional. You can probably make a reasonable guess given that you already know the (one-dimensional) irreps of $SO(2)$.]

6.3 Groups $SO(3)$ and $O(3)$

⨀ The group $SO(3)$ consists of 3×3 orthogonal matrices with determinant $+1$, while $O(3)$ includes in addition the 3×3 orthogonal matrices with determinant -1. (The determinant of a real orthogonal matrix has to be either $+1$ or -1; there are no other possibilities.)

⨀ A convenient way to represent the elements of $SO(3)$ is to write them in the form

$$R(\boldsymbol{\omega}) = e^{-i\boldsymbol{\omega}\cdot\boldsymbol{K}}, \quad \boldsymbol{\omega} = (\omega_x, \omega_y, \omega_z), \tag{33}$$

where $\omega_x, \omega_y, \omega_z$ are real numbers, and $\boldsymbol{\omega}$ represents a (right handed) rotation by an angle $\omega = |\boldsymbol{\omega}| = \sqrt{\omega_x^2 + \omega_y^2 + \omega_z^2}$ about an axis $\boldsymbol{n} = \boldsymbol{\omega}/\omega$, and $\boldsymbol{K} = (K_x, K_y, K_z)$ is the triple of matrices

$$K_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad K_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad K_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{34}$$

• Writing (33) with i in the exponent, and then using pure imaginary matrices in (34) may seem, and indeed is, a little odd. The point is that in quantum mechanics it is customary to write rotations as operators in the general form

$$R(\boldsymbol{\omega}) = e^{-i\boldsymbol{\omega}\cdot\boldsymbol{J}} \tag{35}$$

where $\boldsymbol{J} = (J_x, J_y, J_z)$ is the triple of Hermitian angular momentum operators in units of $\hbar$ (or setting $\hbar = 1$), and so (33) is written this way, but with $\boldsymbol{K}$ in place of $\boldsymbol{J}$.

⊙ The group SO(3) is a continuous group described by three real parameters, the components of $\boldsymbol{\omega}$, confined to the sphere

$$\omega = |\boldsymbol{\omega}| \leq \pi. \tag{36}$$

However, it is important to note that this manifold is "periodically connected" in the sense that two points at the ends of a diameter, $\boldsymbol{\omega}$ and $-\boldsymbol{\omega}$ when $\omega = \pi$, represent the same rotation, the same 3×3 matrix.

⋆ Exercise. Work this out for the case $\boldsymbol{\omega} = (0, 0, \pm\pi)$.

• Thus traveling continuously outwards from the center of the sphere along a radius towards the north pole will eventually result in a "hop" from the north to the south pole—both poles represent the same rotation matrix—and then moving back from the south pole towards the center of the sphere.

⊙ The group $O(3)$ contains the $SO(3)$ matrices just described and also the matrices obtained from these by multiplying by -1 or, perhaps better, $-I$, the matrix representing the parity operator Π that simultaneously maps x to $-x$, y to $-y$, and z to $-z$. Hence the manifold that describes it is disconnected (clearly there is no way for the determinant to change continuously from $+1$ to -1) and consists of the $\boldsymbol{\omega}$ sphere described above along with a copy of it that represents the improper rotations: a rotation combined with a reflection.

⋆ Exercise. A special case of an improper rotation is a reflection in a two-dimensional plane that passes through the origin. E.g., if the plane is perpendicular to the z axis, the corresponding matrix is:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Show that such reflections only constitute a special subset of $O(3)$, and there are lots of other improper rotations.

⊙ An alternative way to parametrize $SO(3)$ is to use the *Euler angles*, three real angles which we shall denote by α, β and γ. Unfortunately they can be, and are, defined in many different ways. The following is one way to do it. First rotate by α about the z axis. Next by β around the y axis. Next by γ about the z axis. The result in the notation used in (33) is the product:

$$e^{-i\gamma K_z} e^{-i\beta K_y} e^{-i\alpha K_z}. \tag{37}$$

• Warning! these matrices do not commute, and so (37) is *not* (leaving aside special cases) the same as $-i\boldsymbol{\omega} \cdot \boldsymbol{K}$ with $\boldsymbol{\omega} = (\alpha, \beta, \gamma)$.

• Whether one uses (33) or (37) is a matter of convenience. In either case one has three real parameters, so a three-dimensional manifold.

• Of course the additional matrices in $O(3)$ are obtained by multiplying the $SO(3)$ matrices by -1, whether one uses the $\boldsymbol{\omega}$ or the Euler angle notation for the latter.

6.4 Group $SU(2)$

⊙ The group $SU(2)$ consists of all unitary 2×2 matrices with determinant $+1$; this last condition is what the S ("special") in $SU(2)$ stands for. It turns out that all such matrices can be written in the form

$$R(\boldsymbol{\omega}) = e^{-i\boldsymbol{\omega}\cdot\boldsymbol{\sigma}/2}, \tag{38}$$

which is of the "standard" form (35) when one writes, as appropriate for spin-half, $\boldsymbol{J} = \boldsymbol{\sigma}/2$; $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the "vector" of Pauli matrices (3).

• While formally (38) looks like (33), there is a subtle difference, which can be explored by assuming that $\boldsymbol{\omega} = (0, 0, \phi)$ corresponding to a rotation about the z axis, in which case the explicit matrix is

$$R(0, 0, \phi) = \begin{pmatrix} e^{-i\phi/2} & 0 \\ 0 & e^{+i\phi/2} \end{pmatrix}. \tag{39}$$

Start at $\phi = 0$ where $R = I$ is the identity operator, and increase it continuously to π, at which point one has $R = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$. But this is *not* the same as for $\phi = -\pi$, which is $R = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$, unlike the case of $SO(3)$ given by (33). Indeed, it is easy to see that

$$R(0, 0, \phi + 2\pi) = -R(0, 0, \phi), \tag{40}$$

so that regarded as a function of ϕ we have something with a period of 4π rather than 2π. The analogous thing happens upon moving outward from $\boldsymbol{\omega} = 0$ along some other axis: when $\omega = \pi$ one comes back to the opposite side (antipode) of the $\omega \leq \pi$ sphere, but with a minus sign.

• Thus one can think of $SU(2)$ as parametrized by two spheres of radius π, but they form a single connected manifold, quite unlike $O(3)$; I like to think of them as lying on top of each other: say a sphere containing red points and another containing green points. Moving out through the surface of one sphere one finds oneself in the other sphere. For an unambiguous label of group elements one could use, for example

$$(\omega_x, \omega_y, \omega_z, \nu); \quad \nu = +1 \text{ or } -1, \tag{41}$$

where

$$R(\omega_x, \omega_y, \omega_z, +1) = -R(\omega_x, \omega_y, \omega_z, -1), \tag{42}$$

and $R(\boldsymbol{\omega}, +1) = R(-\boldsymbol{\omega}, -1)$ when $|\boldsymbol{\omega}| = \pi$.

⊙ There is a 2-to-1 homomorphism from $SU(2)$ to $SO(3)$ in which both of the complex 2×2 matrices $R(\boldsymbol{\omega}, +1)$ and $R(\boldsymbol{\omega}, -1)$ just defined map onto the real 3×3 matrix defined in (33) using $\boldsymbol{K}$ as written in (34). In particular both $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$ are mapped to the 3×3 identity matrix I. So $SU(2)$ and $SO(3)$ are very closely related, but not quite the same thing.

• An important consequence of this homomorphism is that *every representation of $SO(3)$ is also a representation of $SU(2)$*. The reason is that a representation is always of homomorphism of a group to a set of linear maps (or matrices), so by composing the $SU(2)$ to $SO(3)$ homomorphism with that from $SO(3)$ to its representation one obtains a representation of $SU(2)$. The converse is not true: there are representations of $SU(2)$ which are *not* representations of $SO(3)$, at least in the ordinary sense. (They are sometimes called double-valued representations, or else projective representations of $SO(3)$.) In a certain sense the simplest approach is to think of "rotations" as used in quantum mechanics as corresponding to the "bigger" $SU(2)$ group.

7 Irreducible Representations of Rotations

• The theory of representations of $SU(2)$, $SO(3)$ and $O(3)$ constitutes a large subject. Here are some key facts.

⊙ The inequivalent irreducible representations of $SU(2)$ carry a label j, which can take on the values $0, 1/2, 1, 3/2, \ldots$. All nonnegative integers and half-odd integers ("half-integers" for short). Representation j has dimension $2j+1$, so consists of $(2j+1) \times (2j+1)$ matrices.

⊙ The elegant approach to deriving representations uses algebraic properties of the angular momentum operators, in particular their commutation relations:

$$[J_x, J_y] = iJ_z, \quad [J_y, J_z] = iJ_x, \quad [J_z, J_x] = iJ_y. \tag{43}$$

◦ Using these relations one can show that

$$J^2 = J_x^2 + J_y^2 + J_z^2, \tag{44}$$

the "total angular momentum operator," commutes with J_x, J_y and J_z.

• A set of three $n \times n$ matrices that satisfy (43) is said to be an irreducible representation provided there is no similarity transformation that makes all three of them simultaneously block diagonal. Given such an irreducible representation of the angular momentum operators, exponentiating them using (35) yields an irreducible representation of $SU(2)$.

⊙ There is a standard convention for representing the angular momentum operators for irrep j as $(2j+1) \times (2j+1)$ matrices, and it is worked out in many places. One uses an orthonormal basis of kets $|jm\rangle$, where j labels the irrep that one is interested in, and m takes on the $2j+1$ values $-j, -j+1, \ldots j-1, j$. Note that m takes on integer values if j is an integer, and half-integer values when j is a half integer.

• The standard basis is defined so that

$$J_z|jm\rangle = m|jm\rangle, \quad \langle jm'|J_+|jm\rangle = \langle jm|J_-|jm'\rangle = \sqrt{j(j+1) - mm'}\, \delta_{m',m+1}, \tag{45}$$

where $J_+ = J_x + iJ_y$ and its adjoint is $J_- = J_x - iJ_y$. In addition it is the case that

$$J^2|jm\rangle = j(j+1)|jm\rangle, \tag{46}$$

so J^2 is simply $j(j+1)I$ in irrep j.

• Matrices for a fixed j are written with rows and columns labeled by m in decreasing order, thus $m = 1, 0, -1$ in the case $j = 1$.

• For $j = 1/2$ the standard basis gives $J_x = \sigma_x/2, J_y = \sigma_y/2, J_z = \sigma_z/2$.

⋆ Exercise. Show this.

⊙ The irreps of $SO(3)$ are the $SU(2)$ irreps for integer values of j. One often replaces j with the symbol l. The dimension of irrep l is thus $2l+1$.

⊙ The irreps of $O(3)$ can be labeled as (l, p), where l is a nonnegative integer corresponding to the $j = l$ irrep of $SU(2)$, and p (parity) is $+1$ or -1 depending on whether the reflection operator Π is represented by I or by $-I$. In either case the dimension of the irrep is $2l+1$.