Ph195b lecture notes for 2/27/02

Symmetry groups and group representations

[Merzbacher Ch. 17 §3]

Let's begin by reviewing the algebraic notion of a *group*.

A group consists of a set of elements (of arbitrary type), together with a multiplication rule, which satisfy the following properties:

1. The set must be closed under its multiplication rule. That is, if a and b are elements of the group, ab and ba must also be in the group. If $ab = ba$ for every pair of elements, the group is called 'Abelian' (or 'commutative').
2. The multiplication rule must be associative, that is, $(ab)c = a(bc)$.
3. The set must contain an identity element e, such that $ae = ea = a$ for all a.
4. Each element a must have an inverse a^{-1}, such that $a^{-1}a = aa^{-1} = e$.

A simple example of an Abelian group is the pair of numbers $\{-1, 1\}$ under normal multiplication. Another example is the set of matrices

$$\left\{ \begin{array}{l} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \\ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \end{array} \right\}$$

under matrix multiplication, which form a non-commutative group. Note that the pair of matrices

$$\left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right\}$$

form an Abelian group (under matrix multiplication) that is *isomorphic* to our first example. The essential structure of a group is its multiplication 'table,' which for the example $\{a \leftrightarrow -1, e \leftrightarrow 1\}$ is clearly

$$\begin{aligned} aa &= e \\ ae &= a \\ ea &= a \\ ee &= e \end{aligned} .$$

We see that the pair of matrices has exactly the same multiplication table, under the obvious mapping

$$\left\{ a \leftrightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, e \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right\}.$$

In this sense it is really a 'representation' of the same group, which by mathematical convention is generally referred to as C_2. We shall use the term *linear representation* (or simply, representation) to mean an association (not necessarily one-to-one) between each element a in a group and a matrix $D(a)$ that preserves the multiplication rule:

$$D(a)D(b) = D(ab).$$

So far we have seen how C_2 can be represented by 1×1 real matrices (numbers) and 2×2 real matrices. One often speaks of these as being representations 'on' the vector spaces $\mathbf{R}^1$ and $\mathbf{R}^2$, respectively.

To emphasize the abstract nature of the concept, let's think about the *dihedral group*, denoted D_2. Its multiplication table is

	e	a	b	c
e	e	a	b	c
a	a	e	c	b
b	b	c	e	a
c	c	b	a	e

This is clearly Abelian. With reference to the following figure [Wu-Ki Tung, *Group Theory in Physics* (World Scientific, 1985)]

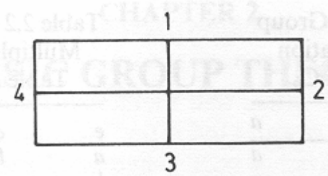

Fig. 2.1 A configuration with D_2 symmetry.

we can associate group elements with symmetries of the rectangle,

- e leave the figure unchanged,
- a reflect through the vertical axis $1-3$,
- b reflect through the horizontal axis $2-4$,
- c rotate (in the plane) about the center point by angle π.

We can easily find a representation of this group on $\mathbf{R}^2$,

$$e \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad b \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$a \leftrightarrow \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad c \leftrightarrow \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Sometimes we find that a group representation 'contains' smaller representations within it. For example, consider our representation of C_2 on $\mathbf{R}^2$, with

$$\left\{ a \leftrightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, e \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right\}.$$

We first note that a linear change of basis for the representing vector space preserves group representations, since under

$$D(a) \mapsto S^{-1}D(a)S,$$

the mapping property

$$D(a)D(b) = D(ab)$$

transforms according to

$$\begin{aligned} S^{-1}D(a)SS^{-1}D(b)S &= S^{-1}D(ab)S, \\ S^{-1}D(a)D(b)S &= S^{-1}D(ab)S, \\ D(a)D(b) &= D(ab). \end{aligned}$$

Two representations related by such a similarity transform are said to be equivalent. If in our example we switch to the basis

$$\left\{ \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \right\},$$

for $\mathbf{R}^2$, our C_2 representation maps to

$$\left\{ a \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, e \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right\}.$$

This clearly still respects the C_2 multiplication table

$$\begin{matrix} e & a \\ a & e \end{matrix}.$$

We see that the $\{a \leftrightarrow -1, e \leftrightarrow 1\}$ representation on $\mathbf{R}^1$ actually appears as the lower-right 'corner' of the $\mathbf{R}^2$ representation, living in its own little subspace and constituting a 1×1 *subrepresentation* of the 2×2 one. What about the upper-left subspace? Here we find the *degenerate* representation $\{a \leftrightarrow 1, e \leftrightarrow 1\}$ of C_2 on $\mathbf{R}^1$, which is not a terribly useful representation but a valid one none-the-less.

In general, it is often possible to take an $n \times n$ representation and find a basis in which all the constituent matrices assume block-diagonal form

$$D_n(a) = \begin{pmatrix} D_1(a) & 0 & 0 & \cdots \\ 0 & D_2(a) & 0 & \cdots \\ 0 & 0 & D_3(a) & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

where $D_1(a)$ has dimensions $n_1 \times n_1$, $D_2(a)$ has dimensions $n_2 \times n_2$, etc. and $n_1 + n_2 + n_3 + \cdots = n$. Each of the sets of matrices $\{D_i(a)\}$ then forms a subrepresentation of the original one, which is therefore said to be *reducible*, and we write

$$D_n = D_1 \oplus D_2 \oplus D_3 \oplus \cdots,$$

i.e., each $D_n(a)$ is the direct sum of the $D_i(a)$. A representation that cannot be broken down in this way is called an irreducible representation, or *irrep* for short. Up to equivalence transformations, the decomposition of a representation into irreps is unique.

It is important to appreciate that we can use the direct sum to build larger representations out of smaller ones. For example, working again with representations of C_2, and denoting our previous representations as d_1 (on $\mathbf{R}^1$) and d_2 (on $\mathbf{R}^2$), we have

$$d_1 \oplus d_1 : \quad \left\{ a \leftrightarrow \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, e \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right\},$$

$$d_1 \oplus d_2 : \quad \left\{ a \leftrightarrow \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, e \leftrightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\},$$

$$d_2 \oplus d_2 : \quad \left\{ a \leftrightarrow \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, e \leftrightarrow \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \right\},$$

$$d_1 \oplus d_1 \oplus d_1 : \quad \left\{ a \leftrightarrow \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, e \leftrightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\},$$

and so on.

Another important way to build larger representation is by taking the tensor product (also known as direct product) of smaller ones. Recall from first term that for a pair of matrices

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots \\ a_{21} & a_{22} & a_{23} & \cdots \\ a_{31} & a_{32} & a_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad B = \begin{pmatrix} b_{11} & b_{12} & b_{13} & \cdots \\ b_{21} & b_{22} & b_{23} & \cdots \\ b_{31} & b_{32} & b_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

the tensor product $A \otimes B$ is given by

$$\begin{pmatrix} a_{11}B & a_{12}B & a_{13}B & \cdots \\ a_{21}B & a_{22}B & a_{23}B & \cdots \\ a_{31}B & a_{32}B & a_{33}B & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

For 2×2 matrices, *e.g.*, we can write more concretely

$$A \otimes B = \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}.$$

We can verify that $d_2 \otimes d_2$ for our C_2 example still constitutes a valid representation, which happens to be equivalent to $d_2 \oplus d_2$.

$$a \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad e \leftrightarrow \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$a^2 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = e.$$

General proofs regarding composite representations can be found in standard textbooks on group representation theory (such as Tung, referenced above).

A useful theorem for recognizing irreducible representations is given by Schur's Second Lemma, which states that [Merzbacher, p. 421] *if the matrices $D(a)$ form an irreducible representation of a group and if a matrix M commutes with all $D(a)$,*

$$[M, D(a)] = 0 \qquad \text{for every } a$$

then M is a multiple of the identity matrix. Hence, if for a given representation we can find a commuting matrix C that is not simply proportional to the identity, we know that the representation is reducible. In general (provided C is normal), there will be some change of basis (corresponding to diagonalizing C) that takes C to a matrix of the form

$$C \mapsto \begin{pmatrix} c_1 I_1 & 0 & 0 & \cdots \\ 0 & c_2 I_2 & 0 & \cdots \\ 0 & 0 & c_3 I_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

where the I_i are identity matrices of dimension $n_i \times n_i$. It follows that each of the n_i –dimensional subspaces constitutes an irreducible subrepresentation.

Representations of the Rotation Group $R(3)$

It is easy to see that the set of all possible rotations in three-dimensional Euclidean space form a group. Any particular member of the group may be specified by its angle and axis of rotation, group multiplication corresponds to the successive application of the two rotations, and the identity element can be chosen as any rotation by zero angle (about any axis). Closure and associativity clearly hold, and this group $R(3)$ is clearly not commutative.

Let us consider the association

$$(\hat{n}, \varphi) \mapsto \exp\left(\frac{-i}{\hbar}\hat{n} \cdot \vec{\mathbf{J}}\varphi\right),$$

where $(\hat{n}, \varphi) \in R(3)$ is a rotation about axis $\hat{n}$ by angle φ ($\hat{n}$ is assumed to be a unit vector) and $\vec{\mathbf{J}}$ is a vector of angular momentum operators $(\mathbf{J}_x, \mathbf{J}_y, \mathbf{J}_z)$. We have previously introduced the idea that any set of three operators $\{\mathbf{J}_x, \mathbf{J}_y, \mathbf{J}_z\}$ satisfying the fundamental commutation relations

$$[\mathbf{J}_x, \mathbf{J}_y] = i\hbar\mathbf{J}_z, \quad [\mathbf{J}_y, \mathbf{J}_z] = i\hbar\mathbf{J}_x, \quad [\mathbf{J}_z, \mathbf{J}_x] = i\hbar\mathbf{J}_y,$$

are legitimate angular momentum operators, with two familiar examples being $\vec{\mathbf{J}} = \vec{\mathbf{L}} = \vec{\mathbf{r}} \times \vec{\mathbf{p}}$ (orbital angular momentum) and $\vec{\mathbf{J}} = \vec{\mathbf{S}}$ (spin-1/2). The reason for this now becomes clear, as any set of generators $\{\mathbf{J}_x, \mathbf{J}_y, \mathbf{J}_z\}$ satisfying the above commutation relations can be used in the above association between rotations and Hilbert-space operators to yield a valid representation of $R(3)$. Preservation of the appropriate multiplication table is guarenteed by the commutation relations and the operator-exponential structure of the association. The proof of this is straightforward but quite tedious – we actually saw a sketch of it at the end of the last lecture, but I refer you to Cohen-Tannoudji, Diu, and Laloe Complement B_{VI} for a more patient and careful treatment.

In the case of spin-1/2, we clearly have a 2×2 representation of $R(3)$ on $\mathbf{C}^2$ (the two-dimensional complex vector space, not the two-element group!), as the generators are simply proportional to the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Application of the association law yields

$$(\hat{n}, \varphi) \mapsto \begin{pmatrix} \cos\frac{\varphi}{2} - in_z \sin\frac{\varphi}{2} & (-in_x - n_y)\sin\frac{\varphi}{2} \\ (-in_x + n_y)\sin\frac{\varphi}{2} & \cos\frac{\varphi}{2} + in_z \sin\frac{\varphi}{2} \end{pmatrix},$$

where $\hat{n} = (n_x, n_y, n_z)$. When the state of a spin-1/2 system is expressed in the σ_z basis, these unitary matrices are the Hilbert-space operators corresponding to rotations in the $3D$ coordinate space.

In the case of orbital angular momentum, things would seem to be much more complicated since the underlying Hilbert space is infinite dimensional. But if you think about it, we have already seen that the $\vec{\mathbf{r}} \times \vec{\mathbf{p}}$ representation decomposes into a succession of finite-dimensional representations! These correspond to the subspaces of given j, with dimension $2j + 1$. For example, we find a three-dimensional representation of the rotation group with $j = 1$. The basis vectors (kets) for the representing vector space are

$$|1;+1\rangle \leftrightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |1;0\rangle \leftrightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |1;-1\rangle \leftrightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

with angular momentum operators

$$\mathbf{J}_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \mathbf{J}_+ = \hbar\begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{J}_- = \hbar\begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix},$$

$$\mathbf{J}_x = \frac{1}{2}(\mathbf{J}_+ + \mathbf{J}_-), \qquad \mathbf{J}_y = \frac{-i}{2}(\mathbf{J}_+ - \mathbf{J}_-).$$

Formally, we can accomplish the desired decomposition by noting that on the entire state space for particle motion in three kinetic dimensions,

$$\mathbf{J}^2 = \mathbf{J}_x^2 + \mathbf{J}_y^2 + \mathbf{J}_z^2$$

commutes with each of the generators $\{\mathbf{J}_x, \mathbf{J}_y, \mathbf{J}_z\}$. Because of this, it also commutes with every element

$$(\hat{n}, \varphi) \mapsto \exp\left(\frac{-i}{\hbar}\hat{n} \cdot \vec{\mathbf{J}}\varphi\right)$$

in the infinite-dimensional representation of $R(3)$. But we also know that it is diagonal, but not proportional to the identity, in the $|j;m\rangle$ basis:

$$\mathbf{J}^2|j;m\rangle = j(j+1)\hbar^2|j;m\rangle.$$

Hence we can invoke Schur's Second Lemma to show that the subspace spanned by the $2j+1$ states with given j and $-j \le m \le j$ forms a subrepresentation (an irrep, in fact!) of $R(3)$. When used in this capacity, $\mathbf{J}^2$ is referred to as a *Casimir operator* for $R(3)$.

From the point of view of Quantum Mechanics, the important point is that the restrictions of $\{\mathbf{J}_x, \mathbf{J}_y, \mathbf{J}_z\}$, and all polynomials thereof (including the rotation operators) leave subspaces of constant j invariant:

$$\mathbf{J} \leftrightarrow \begin{pmatrix} J(0) & 0 & 0 & \cdots \\ 0 & J(1) & 0 & \cdots \\ 0 & 0 & J(2) & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

where $J(0)$ is a number, $J(1)$ is a 3×3 matrix, $J(2)$ is a 5×5 matrix, etc. Hence any time we are working with a Hamiltonian that commutes with $\mathbf{J}^2$,

$$\left[\mathbf{H}, \mathbf{J}^2\right] = 0,$$

we can think of j as a good quantum number and use finite-dimensional representations of operators within the appropriate subspaces. We'll see more of this soon, when we start to solve the Schrödinger Equation with spherically-symmetric $3D$ potentials.

Addition of Angular Momenta

Say we have a pair of systems, with angular momenta j_1 and j_2. Then we may describe these individually by states in Hilbert spaces of dimension $2j_1+1$ and $2j_2+1$, respectively. The joint state space for these systems, if we couple them, is given by the tensor product space of dimension $(2j_1+1)(2j_2+1)$. This generates a tensor-product representation for $R(3)$,

$$(\hat{n},\varphi) \mapsto \exp\left(\frac{-i}{\hbar}\hat{n}\cdot\vec{\mathbf{J}}_1\varphi\right)\otimes\exp\left(\frac{-i}{\hbar}\hat{n}\cdot\vec{\mathbf{J}}_2\varphi\right)$$
$$= \exp\left(\frac{-i}{\hbar}\hat{n}\cdot\left(\vec{\mathbf{J}}_1\otimes\mathbf{1}^2+\mathbf{1}^1\otimes\vec{\mathbf{J}}_2\right)\varphi\right),$$

where $\vec{\mathbf{J}}_1$ is the vector of angular momentum operators for system 1 and $\vec{\mathbf{J}}_2$ for system 2, $\mathbf{1}^1$ is the identity operator on system 1 and $\mathbf{1}^2$ is the identity operator on system 2. The operators

$$\vec{\mathbf{J}} \equiv \vec{\mathbf{J}}_1\otimes\mathbf{1}^2+\mathbf{1}^1\otimes\vec{\mathbf{J}}_2$$

can be shown to satisfy the required commutation relations and therefore constitute a valid set of angular momentum operators, themselves. As in the past, we will generally drop implied tensor-products for the coupled system and write, *e.g.*, $\vec{\mathbf{J}} = \vec{\mathbf{J}}_1 + \vec{\mathbf{J}}_2$.

If for example $j_1 = 1/2$ and $j_2 = 1$, the tensor-product representation will have dimension $(2)(3) = 6$. As we shall see next time, however, this composite representation does not correspond to the irrep with $j = 5/2$, but rather may be decomposed into the direct sum of irreps with $j = 1/2$ and $j = 3/2$. We see that this is plausible since the dimensions of these irreps add up to $2 + 4 = 6$. Hence, even for the coupled system we anticipate that the state space will break down into 2 – and 4 –dimensional subspaces that are invariant under the action of angular momentum operators and anything else (such as a spherically-symmetric Hamiltonian) that commutes with $\mathbf{J}^2$.