7 Continuous Group

7.2 SO(3)

This is the group of three dimensional real orthogonal matrices with +1 determinant. This set of matrices describe rotation of a three dimensional real vector space. Even though it is just one dimension up from $SO(2)$, it is much more complicated but also much more interesting!

First, $SO(3)$ is not abelian any more. Imagine we perform a rotation around the z axis first by an angle θ, the transformation of the $3D$ vector space is given by

$$R_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{1}$$

Next let's perform a rotation around x axis by an angle θ', the transformation of the $3D$ vector space is given by

$$R_x(\theta') = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta' & -\sin\theta' \\ 0 & \sin\theta' & \cos\theta' \end{pmatrix} \tag{2}$$

Direct calculation shows that $R_z(\theta)R_x(\theta') \neq R_x(\theta')R_z(\theta)$ for general θ and θ'. Similar to the case of $SO(2)$, these three dimensional matrices provide one particular representation of the $SO(3)$ group, but the group may have other representations. This three dimensional representation is special in that it is faithful and irreducible. As a nonabelian group, $SO(3)$ can have higher dimensional irreps, which we are going to discuss later.

Infinitesimal generators

First, let us try to understand what are the infinitesimal generators of $SO(3)$. Following the discussion of $SO(2)$, it is easy to see that to generate rotation around z axis, the infinitesimal generator is

$$L_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{3}$$

such that $R_z(\theta) = e^{-i\theta L_z}$. Similarly, we find that

$$L_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad L_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \tag{4}$$

such that $R_x(\theta) = e^{-i\theta L_x}$, $R_y(\theta) = e^{-i\theta L_y}$. L_x, L_y, L_z each generate a subgroup of rotation around x, y and z axes respectively.

Are L_x, L_y, L_z enough to generate all $SO(3)$ transformations?

Euler's rotation theorem says: any transformation in $SO(3)$ is equivalent to a single rotation about some axis for a certain angle. It can be shown (Jones page 102-103) that such rotation operation can be written in the form

$$R_{\vec{n}}(\theta) = e^{-i\theta(n_x L_x + n_y L_y + n_z L_z)} = e^{-i\theta L_{\vec{n}}} \tag{5}$$

Therefore, the linear combination of L_x, L_y and L_z gives the infinitesimal generator of all transformations in $SO(3)$, which is the angular momentum operator in direction $\vec{n}$. The inverse of this operation corresponds to rotation around the same axis but with opposite angle $R_{\vec{n}}^{-1}(\theta) = e^{i\theta X_{\vec{n}}}$.

The vector space of linear combinations of L_x, L_y, and L_z leads to the most important concept in describing the set of continuous groups we are interested in.

$SO(3)$ (and also $SO(2)$) is an example of a Lie group. Its infinitesimal generators form a Lie algebra. The Lie algebra is usually denoted with lower case letters of the name of the group. For example, the Lie algebra of the $SO(2)$ group is $so(2)$ and the Lie algebra of $SO(3)$ is $so(3)$.

There are two important structures of this algebra:

(1) it is a real vector space. That is, the linear combination of two infinitesimal generators is (linearly proportional to) an infinitesimal generator;

(2) The commutator of two infinitesimal generators $[X_i, X_j] = X_i X_j - X_j X_i$ is (linearly proportional to) an infinitesimal generator.

Comment:

1. By focusing on the infinitesimal generators, we reduce the study of a continuous group with an infinite number of elements to the study of a finite set, the basis of the Lie algebra.

2. In $SO(3)$, L_x, L_y, L_z form the basis of the vector space. We have shown above that (1) is true for $SO(3)$. Let's now see that (2) is also true. First $[L_i, L_i] = 0$ which is the infinitesimal generator for doing nothing because $e^{i\theta 0} = I$.

$$[L_x, L_y] = iL_z, [L_y, L_z] = iL_x, [L_z, L_x] = iL_y \tag{6}$$

From which we can show that for any two linear combinations of L_x, L_y, L_z, we have

$$[\vec{n}^a \cdot \vec{L}, \vec{n}^b \cdot \vec{L}] = i(\vec{n}^a \times \vec{n}^b) \cdot \vec{L} \tag{7}$$

3. Notice that because in general L_i's do not commute, $e^{i\theta \sum_i n_i L_i} \neq \prod_i e^{i\theta n_i L_i}$.

4. The commutator can be thought of as a composition rule between the infinitesimal generators, mapping two such generators to a third one. This composition rule is anti-commuting, $[X_i, X_j] = -[X_j, X_i]$. It satisfies the Jacobi Identity

$$[[X, Y], Z] + [[Y, Z], X] + [[Z, X], Y] = 0 \tag{8}$$

5. The commutator between the infinitesimal generators is very useful in determining the conjugacy classes of the group. For $SO(3)$ we are going to find that rotation operations around different axes with the same angle are conjugate to each other. That is,

$$e^{i\phi\vec{n}_2\cdot\vec{L}} e^{i\theta\vec{n}_1\cdot\vec{L}} e^{-i\phi\vec{n}_2\cdot\vec{L}} = e^{i\theta\vec{n}_3\cdot\vec{L}} \tag{9}$$

Physically this is very intuitive. We can imagine that $e^{i\phi\vec{n}_2\cdot\vec{L}}$ and $e^{-i\phi\vec{n}_2\cdot\vec{L}}$ maps the vector $\vec{n}_1$ to $\vec{n}_3$ and back. Then under this mapping, the rotation around axis $\vec{n}_1$ for angle θ is mapped to rotation around axis $\vec{n}_3$ for angle θ.

We are not going to derive this result in class, but we are going to work it out in the homework.

6. The conjugacy classes of $SO(3)$ then consist of rotation through the same angle about different axes and can be labelled simply by that angle θ. Correspondingly, characters are just a function of θ. In the three dimensional special orthogonal representation, we have

$$\chi = 2\cos(\theta) + 1 \tag{10}$$

which can be verified directly for $R_x(\theta)$, $R_y(\theta)$ and $R_z(\theta)$.

Irreducible representations

Now let's see what irreps the group $SO(3)$ has. There is an infinite number of them, as you might have expected from the continuous nature of this group. Instead of trying to find irreps of the group elements, we can just find irreps of the infinitesimal generators (the algebra). Then by taking the exponetial, we can recover the group elements.

That is, we are looking for irreducible representations of L_x, L_y, L_z such that

1. L_x, L_y, L_z are finite dimensional Hermitian operators.

2. they satisfy the relation $[L_a, L_b] = i\epsilon_{abc}L_c$, where $\epsilon_{abc} = 1$ if $\{abc\}$ can be obtained from $\{xyz\}$ by a cyclic permutation, $\epsilon_{abc} = -1$ if $\{abc\}$ can be obtained from $\{xyz\}$ by a cyclic permutation and an exchange and $\epsilon_{abc} = 0$ otherwise.

3. once exponentiated, they give rise to the $SO(3)$ group. (This requirement may seem redundant if the previous two are satisfied. But in fact it is not, as we are going to see later on.)

In physics, this exercise is called 'finding the orbitals of an electron in a Hydrogen atom'. Rotation invariance around z axis in the Hydrogen atom implies that every orbit is labeled by a particular value of angular momentum J_z in the z direction. If we take into account the full rotation symmetry of the Hydrogen atom in three dimensional space, then the orbits should be labelled by irreps of the $SO(3)$ group, not just the $SO(2)$ group, and they transform under $SO(3)$ rotation as an irrep.

The first thing to define for an irrep is the 'Casimir Operator': An operator which commutes with all the elements of a Lie group.

Comments:

1. According to Schur's Lemma, the Casimir Operator is proportional to identity on the irrep.

2. An equivalent requirement is that, the Casimir Operator commute with all infinitesimal generators.

3. For $SO(3)$, the Casimir Operator is denoted as L^2 and one can check that it can be obtained from $L^2 = L_x^2 + L_y^2 + L_z^2$. For the 3D special orthogonal representation, $L^2 = 2I_3$. Physically, it has the meaning of the total magnitude of the orbital angular momentum of the electron. All vectors

of an irrep are eigenvectors of L^2 with the same eigenvalue. This eigenvalue provides a one to one labelling of the equivalence class of irreps of $SO(3)$.

Previously when we talked about irreps, we always talked about the equivalence class of them without choosing a particular basis and hence a particular form of the representation matrices. With $SO(3)$, physicist prefer to use a special basis and we are going to write everything down using this basis. Recall that L_x, L_y and L_z do not commute. Therefore, we cannot find a common basis for all three of them. Instead, we just use the eigenstates of L_z as the basis to write down irreps. That is, the basis states are common eigenvectors of L^2 and L_z. This is possible because L^2 and L_z commute.

So what are the eigenstates of L_z in a finite dimensional irrep? Suppose that state $|m\rangle$ is one such eigenstate satisfying

$$L_z|m\rangle = m|m\rangle \tag{11}$$

Then under rotation around z axis, this state $|m\rangle$ acquires a phase factor

$$e^{-i\theta L_z}|m\rangle = e^{-i\theta m}|m\rangle \tag{12}$$

Because $\theta = 2\pi$ rotation is the same as the identity transformation, we have $e^{-i2\pi m} = 1$. That is, the eigenvalues of L_z are integers. Similarly the eigenvalues of L_x and L_y are also integers.

In a finite dimensional representation, m has an upper bound. Let's suppose that this maximum value is $j \in \mathbb{Z}_+$ (or $j = 0$). From here, we can derive the whole representation as follows.

Starting from $|j\rangle$, we can go to all other eigenstates of L_z by applying L_x and L_y. In particular, define

$$L_\pm = L_x \pm iL_y \tag{13}$$

as the raising and lowering operators. ${L_\pm}^\dagger = L_\mp$. They earned these names because applying $L_\pm$ on $|m\rangle$ maps it to $|m \pm 1\rangle$.

$$L_z(L_\pm|m\rangle) = L_z(L_x \pm iL_y)|m\rangle = (L_xL_z + iL_y \pm iL_yL_z \pm L_x)|m\rangle = (m \pm 1)L_\pm|m\rangle \tag{14}$$

Now if we apply L_+ to $|j\rangle$ the resulting state should have 0 norm because we assumed that $|j\rangle$ is already the eigenvector with the largest L_z eigenvalue.

$$L_+|j\rangle = (L_x + iL_y)|j\rangle = 0 \tag{15}$$

Because of this, we can see that $|j\rangle$ is an eigenstate of L^2 with eigenvalue $j(j+1)$ because

$$L^2|j\rangle = (L_z^2 + L_x^2 + L_y^2)|j\rangle = (L_z^2 + L_-L_+ + L_z)|j\rangle = j(j+1)|j\rangle \tag{16}$$

Because we know that L^2 is proportional to identity in a particular irrep. Therefore, in this irrep, all states (the $|m\rangle$s and their superpositions) are eigenstates of L^2 with eigenvalue $j(j+1)$.

Now let's apply L_- to $|j\rangle$ and obtain all other eigenstates of L_z with smaller eigenvalues.

$$L_-|j\rangle \propto |j-1\rangle, L_-|j-1\rangle \propto |j-2\rangle, ... \tag{17}$$

There are two questions we need to answer regarding this procedure: 1. what is the normalization of states $L_-|m\rangle$? 2. when does this procedure stop? That is, there is a minimum m in every finite dimensional representation. What is this minimum m given j?

To answer this question, we observe that

$$\langle m|L_+L_-|m\rangle = \langle m|L^2 - L_z^2 + L_z|m\rangle = j(j+1) - m(m-1) \tag{18}$$

Therefore,

$$L_-|m\rangle = \sqrt{j(j+1) - m(m-1)}|m-1\rangle \tag{19}$$

and this procedure stops when $j(j+1) - m(m-1) = 0$, which happens if $m = j+1$ or $m = -j$. Because we know that $m \leq j$, therefore, the only solution is actually $m = -j$, which is the smallest eigenvalue of L_z in this irrep. Similar calculation shows

$$L_+|m\rangle = \sqrt{j(j+1) - m(m+1)}|m+1\rangle \tag{20}$$

In this way, we have found a representation of the infinitesimal generators of $SO(3)$ on a $2j+1$ dimensional vector space with basis vectors

$$|j\rangle, |j-1\rangle, ..., |-j\rangle \tag{21}$$

which transforms under L_+, L_-, L_z as

$$L_z|m\rangle = m|m\rangle, L_+|m\rangle = \sqrt{j(j+1) - m(m+1)}|m+1\rangle, L_-|m\rangle = \sqrt{j(j+1) - m(m-1)}|m-1\rangle \tag{22}$$

Correspondingly

$$\begin{aligned} L_x|m\rangle &= \tfrac{1}{2}(\sqrt{j(j+1) - m(m+1)}|m+1\rangle + \sqrt{j(j+1) - m(m-1)}|m-1\rangle), \\ L_y|m\rangle &= \tfrac{1}{2i}(\sqrt{j(j+1) - m(m+1)}|m+1\rangle - \sqrt{j(j+1) - m(m-1)}|m-1\rangle), \\ L_z|m\rangle &= m|m\rangle, L^2|m\rangle = j(j+1)|m\rangle \end{aligned} \tag{23}$$

Let's see how this looks like in some simple cases.

First, consider the case of $j = 0$. This irrep is one dimensional and the operators are all represented as numbers

$$L_z = 0, L_x = 0, L_y = 0, L^2 = 0 \tag{24}$$

If we exponentiate them, the rotation operators we get are all trivial

$$R_{\vec{n}}(\theta) = e^{-i\theta(n_x L_x + n_y L_y + n_z L_z)} = 1 \tag{25}$$

Next, let's move on to the case of $j = 1$. This irrep is three dimensional with basis states $|1\rangle$, $|0\rangle$, $|-1\rangle$. In matrix form, L_x, L_y, L_z and L^2 read

$$L_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \; L_x = \frac{1}{2}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}, \; L_y = \frac{i}{2}\begin{pmatrix} 0 & -\sqrt{2} & 0 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}, \; L^2 = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \tag{26}$$

We know of another three dimensional representation of $SO(3)$ which is given by the three dimensional special orthogonal matrices. How are these two representations related? If we list the generators of the special orthogonal matrices, we can see that

$$X_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, X_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, X_3 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{27}$$

This is related to the L_x, L_y, L_z given above by a basis transformation

$$S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & i & 0 \end{pmatrix} \tag{28}$$

Therefore, the two three dimensional representations we have seen so far, are equivalent to each other.

Similarly, we can build up representations of five, seven, ... dimensions. Each of them correspond to a different irrep of $SO(3)$. That is, $SO(3)$ has one equivalence class of irrep in every odd dimension, labeled by integer j.