8 Continuous Group

8.2 SO(3)

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, we can just find irreps of the infinitesimal generators (the algebra). Then by taking the exponential, we can recover the group elements.

That is, we are looking for irreducible representations of $X_1, X_2, X_3$ such that

1. $X_1, X_2, X_3$ are finite dimensional Hermitian operators.

2. they satisfy the relation $[X_a, X_b] = i\epsilon_{abc}X_c$, where $\epsilon_{abc} = 1$ if $\{ijk\}$ 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 orbit 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.

So let’s follow the physicists notation. We write $J_x, J_y$ and $J_z$ for $X_1, X_2, X_3$ and look for their irreps.

The first thing to define for an irrep is the ‘Casimir Operator’: An operator which commutes with all the elements of a Lie group is said to be a ‘Casimir Operator’ of that 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 $J^2$ and one can check that it can be obtained from $J^2 = J_x^2 + J_y^2 + J_z^2$. For the 3D special orthogonal representation, $J^2 = 2I_3$. 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 $J^2$ 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 $SO(3)$, physicists prefer to use a special basis and we are going to write everything down using this basis. Recall that $J_x$, $J_y$ and $J_z$ do not commute. Therefore, we cannot find a common basis for all three of them. Instead, we just use the eigenstates of $J_z$ as the basis to write down irreps. That is, the basis states are common eigenvectors of $J^2$ and $J_z$. This is possible because $J^2$ and $J_z$ commute.

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

$$ J_z|m\rangle = m|m\rangle $$

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

$$ e^{-i\theta J_z}|m\rangle = e^{-i\theta m}|m\rangle $$

Because $\theta = 2\pi$ rotation is the same as the identity transformation, we have $e^{-i2\pi m} = 1$. That is, the eigenvalues of $J_z$ are integers. Similarly the eigenvalues of $J_x$ and $J_y$ 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 $J_z$ by applying $J_x$ and $J_y$. In particular, define

$$ J_\pm = J_x \pm i J_y $$

as the raising and lowering operators. $J_\pm$ maps it to $|m \pm 1\rangle$.

$$ J_z(J_\pm|m\rangle) = J_z(J_x \pm i J_y)|m\rangle = (J_xJ_z + i J_y \pm i J_y J_z \pm J_x)|m\rangle = (m \pm 1)J_\pm|m\rangle $$

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

$$ J_+|j\rangle = (J_x+i J_y)|j\rangle = 0 $$

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

$$ J^2|j\rangle = (J_x^2 + J_y^2 + J_z^2)|j\rangle = (J_x^2 + J_y^2 + J_z^2)|j\rangle = j(j + 1)|j\rangle $$

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

Now let’s apply $J_-$ to $|j\rangle$ and obtain all other eigenstates of $J_z$ with smaller eigenvalues.

$$ J_-|j\rangle \propto |j - 1\rangle, J_-|j - 1\rangle \propto |j - 2\rangle, ... $$

There are two questions we need to answer regarding this procedure: 1. what is the normalization of states $J_-|m\rangle$? 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

$$ \langle m| J_+ J_- |m\rangle = \langle m| J^2 - J_z^2 |m\rangle = j(j + 1) - m(m - 1) $$
Therefore,
\[ J_- |m\rangle = \sqrt{j(j+1) - m(m-1)} |m-1\rangle \]  \hspace{1cm} (9)
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 \( J_z \) in this irrep. Similar calculation shows
\[ J_+ |m\rangle = \sqrt{j(j+1) - m(m+1)} |m+1\rangle \]  \hspace{1cm} (10)

In this way, we have found a representation of the infinitesimal generators of \( SO(3) \) on a 2\( j \) + 1 dimensional vector space with basis vectors
\[ |j\rangle, |j-1\rangle, \ldots, |j\rangle \]  \hspace{1cm} (11)
which transforms under \( J_+ \), \( J_- \), \( J_z \) as
\[ J_z |m\rangle = m|m\rangle, J_+ |m\rangle = \sqrt{j(j+1) - m(m+1)} |m+1\rangle, J_- |m\rangle = \sqrt{j(j+1) - m(m-1)} |m-1\rangle \]  \hspace{1cm} (12)
Correspondingly
\[ J_x |m\rangle = \frac{1}{2} (\sqrt{j(j+1) - m(m+1)} |m+1\rangle + \sqrt{j(j+1) - m(m-1)} |m-1\rangle), \]  
\[ J_y |m\rangle = \frac{1}{2} (\sqrt{j(j+1) - m(m+1)} |m+1\rangle - \sqrt{j(j+1) - m(m-1)} |m-1\rangle), \]  
\[ J_z |m\rangle = m|m\rangle, J^2 |m\rangle = j(j+1)|m\rangle \]  \hspace{1cm} (13)

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
\[ J_z = 0, J_x = 0, J_y = 0, J^2 = 0 \]  \hspace{1cm} (14)
If we exponentiate them, the rotation operators we get are all trivial
\[ R_{\vec{n}}(\theta) = e^{-i\theta(n_x J_x + n_y J_y + n_z J_z)} = 1 \]  \hspace{1cm} (15)

Next, let’s move on to the case of \( j = 1 \). This irrep is three dimensional with basis states \( |1\rangle \), \( |0\rangle \), \( |\rangle - 1 \rangle \). In matrix form, \( J_x \), \( J_y \), \( J_z \) and \( J^2 \) read
\[ J_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \]  
\[ J_x = \frac{1}{2} \begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}, \]  
\[ J_y = \frac{i}{2} \begin{pmatrix} 0 & -\sqrt{2} & 0 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}, \]  
\[ J^2 = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \]  \hspace{1cm} (16)

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
\[ X_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ i & 0 & 0 \end{pmatrix}, X_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, X_3 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \]  \hspace{1cm} (17)
This is related to the $J_x, J_y, J_z$ given above by a basis transformation

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

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 $j$.

**Characters**

For an irrep labeled by $j$ as derived above, we can find the character of a conjugacy class labeled by $\theta$ by taking the trace of $R^j_z(\theta)$. In particular

$$J_z = \text{diag}(j, j - 1, ..., -j)$$

Therefore

$$R_z^j(\theta) = \text{diag}(e^{ij\theta}, e^{i(j-1)\theta}, ..., e^{-ij\theta})$$

and the character is

$$\chi^{(j)}(\theta) = \frac{\sin(j + 1/2)\theta}{\sin(\theta/2)}$$

(take $j = 1$ and compare it to the case of the three dimensional special orthogonal representation.)

Are these characters orthogonal to each other? In order to answer the question, we need to define an integration for the group, which integrates over its parameter space. The parameter space of $SO(3)$ is highly nontrivial. First, we can specify every group element by a rotation axis direction $\vec{n}$ and an angle $\theta$. $\vec{n}$ is a unit vector and we can take it to correspond to points on the surface of a unit ball. $\theta$ takes value from $-\pi$ to $\pi$ and we can take it to correspond to the radial direction of the solid ball. However, the parameter space is not the ball because a $\pi$ rotation is the same as a $-\pi$ rotation. Therefore, the two ends of the same diameter should be identified. Therefore, a solid ball with this identification gives the parameter space of $SO(3)$. The geometry and topology of this space is too complicated to discuss here. Instead I will just claim that the integration we want to use is

$$\int_0^{2\pi} \frac{d\theta}{2\pi} (1 - \cos(\theta))$$

and the characters are orthogonal under this integration

$$\langle \chi^{(j)}, \chi^{(j')} \rangle = \int_0^{2\pi} \frac{d\theta}{2\pi} (1 - \cos(\theta)) \frac{\sin(j + 1/2)\theta}{\sin(\theta/2)} \frac{\sin(j' + 1/2)\theta}{\sin(\theta/2)} = \delta_{jj'}$$