Quantum mechanics II, Solutions 10 : Characters and Lie Algebra Basics

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Problem 1 : Irreps of C_{3v}

The aim of this exercise is to consider two representations of the group C_{3v}. We will start by finding the representation R of the group on the vector space $\mathbb{R}^2$. Then we will find the representation P_R of the group on the function space generated by $\Psi_1(\mathbf{r}) = x^2e^{-r}$, $\Psi_2(\mathbf{r}) = y^2e^{-r}$, $\Psi_3(\mathbf{r}) = 2xye^{-r}$. We will show that the representation P_R is reducible. We will establish the connection with the representation R of dimension 2.

1. Consider the vector space $\mathbb{R}^2$ with vectors (x, y). Derive the representation of $R(\sigma_1)$ and $R(C_3)$ in this space. Then deduce the group multiplication table to find $R(u)$, $\forall u \in C_{3v}$. We will assume that this representation is unitary and irreducible, which can be demonstrated by Schur's theorem.
   Solution : The two dimensional representation of C_{3v} is given in the lecture notes as

$$
\begin{aligned}
&e = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\
&C_3 = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \; C_3^2 = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\
&\sigma_1 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \; \sigma_2 = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \; \sigma_3 = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}
\end{aligned}
\tag{1}
$$

2. Consider now the vector space of functions $\mathcal{H}$, generated by functions :

$$
\begin{aligned}
\Psi_1(\mathbf{r}) &= x^2e^{-r} \\
\Psi_2(\mathbf{r}) &= y^2e^{-r} \\
\Psi_3(\mathbf{r}) &= 2xye^{-r}
\end{aligned}
$$

   where $r = |\mathbf{r}| = \sqrt{x^2 + y^2}$, with the scalar product :

$$
\langle \Psi_\alpha | \Psi_\beta \rangle = \int d^2\mathbf{r} \Psi_\alpha^*(\mathbf{r}) \Psi_\beta(\mathbf{r}).
$$

   Written as matrices, the group representation C_{3v} is defined as follows :

$$
P_{R(u)}\Psi(\mathbf{r}) \equiv \Psi(R^{-1}(u)\mathbf{r}), \; \forall u \in \mathcal{H},
$$

   where $R(u)$ are the matrices derived in point (a) (in quantum mechanics, for example, the wave function of a particle obeys this transformation law following a rotation of the reference frame). Show that it is a representation of the group, and that its matrices are not all unitary.

Solution : We write down the transformations for σ_1 and C_3 explicitly. First, we note that the two dimensional representation above is unitary, so $|R(g)\mathbf{r}| = |\mathbf{r}|$ for all $g \in C_{3v}$. We find for the reflection σ_1

$$\begin{aligned} P_{R(\sigma_1)}\Psi_1(\mathbf{r}) &= \Psi(R^{-1}((\sigma_1)\mathbf{r}) = (-x)^2 e^{-r} = \Psi_1(\mathbf{r}), \\ P_{R(\sigma_1)}\Psi_2(\mathbf{r}) &= \Psi(R^{-1}((\sigma_1)\mathbf{r}) = y^2 e^{-r} = \Psi_2(\mathbf{r}), \\ P_{R(\sigma_1)}\Psi_3(\mathbf{r}) &= \Psi(R^{-1}((\sigma_1)\mathbf{r}) = -2xye^{-r} = -\Psi_3(\mathbf{r}) \end{aligned}$$

and hence

$$P_{R(\sigma_1)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{2}$$

For $R^{-1}(C_3) = R(C_3^2)$ we have $R^{-1}(C_3)\mathbf{r} = \begin{pmatrix} -\frac{1}{2}x + \frac{\sqrt{3}}{2}y \\ -\frac{\sqrt{3}}{2}x - \frac{1}{2}y \end{pmatrix}$ and hence

$$\begin{aligned} P_{R(C_3)}\Psi_1(\mathbf{r}) &= \left(-\frac{1}{2}x + \frac{\sqrt{3}}{2}y\right)^2 e^{-r} = \left(\frac{1}{4}x^2 + \frac{3}{4}y^2 - 2\frac{\sqrt{3}}{4}xy\right)e^{-r} = \frac{1}{4}\Psi_1(\mathbf{r}) + \frac{3}{4}\Psi_2(\mathbf{r}) - \frac{\sqrt{3}}{4}\Psi_3(\mathbf{r}) \\ P_{R(C_3)}\Psi_2(\mathbf{r}) &= \left(-\frac{\sqrt{3}}{2}x - \frac{1}{2}y\right)^2 e^{-r} = \left(\frac{3}{4}x^2 + \frac{1}{4}y^2 + 2\frac{\sqrt{3}}{4}xy\right)e^{-r} = \frac{3}{4}\Psi_1(\mathbf{r}) + \frac{1}{4}\Psi_2(\mathbf{r}) + \frac{\sqrt{3}}{4}\Psi_3(\mathbf{r}) \\ P_{R(C_3)}\Psi_3(\mathbf{r}) &= 2\left(-\frac{1}{2}x + \frac{\sqrt{3}}{2}y\right)\left(-\frac{\sqrt{3}}{2}x - \frac{1}{2}y\right)e^{-r} = 2\left(\frac{\sqrt{3}}{4}x^2 - \frac{\sqrt{3}}{4}y^2 - 2\frac{1}{4}xy\right)e^{-r} \\ &= \frac{\sqrt{3}}{2}\Psi_1(\mathbf{r}) - \frac{\sqrt{3}}{2}\Psi_2(\mathbf{r}) - \frac{1}{2}\Psi_3(\mathbf{r}), \end{aligned}$$

We find the matrix representation

$$P_{R(C_3)} = \begin{pmatrix} \frac{1}{4} & \frac{3}{4} & \frac{\sqrt{3}}{2} \\ \frac{3}{4} & \frac{1}{4} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{4} & \frac{\sqrt{3}}{4} & -\frac{1}{2} \end{pmatrix}. \tag{3}$$

We can verify that this is indeed a representation, e.g. $(P_{R(\sigma_1)})^2 = (P_{R(C_3)})^3 = \mathbb{1}$.

3. Show that the representation $P_{R(u)}$ is reducible by identifying an invariant subspace.

   Solution : We note that $v_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$ is an eigenvector of both $P_{R(C_3)}$ and $P_{R(\sigma_1)}$ and hence the subspace spanned by v_1 is invariant under the action of the group.

4. Hence show that the representation R(u) can be written as a direct sum of a 2D and 1D irreducible representations.

   Solution : We first note that $R(u)$ acts trivially on the subspace V_1 spanned by v_1, hence the representation corresponding to this subspace is the trivial one dimensional representation. We find that $\mathcal{H} = V_1 \oplus V_2$ where V_2 is the complemented subspace to V_1 that is spanned by $v_{21} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, v_{22} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$. In this basis, we write down the matrix representations of the representation described above.

$P_{R(\sigma_1)}v_{21} = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix} = -v_{21}$ and $P_{R(\sigma_1)}v_{22} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} = v_{22}$

$P_{R(C_3)}v_{21} = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix} = -\frac{1}{2}v_{21} + \frac{\sqrt{3}}{2}v_{22}$ and $P_{R(C_3)}v_{22} = \begin{pmatrix} -\frac{1}{2} \\ \frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix} = -\frac{\sqrt{3}}{2}v_{21} - \frac{1}{2}v_{22}$ therefore we find

$$\left[P_{R(\sigma_1)}\right]_{V_2} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \tag{4}$$

$$\left[P_{R(C_3)}\right]_{V_2} = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \tag{5}$$

which is equivalent to the two dimensional representation discussed before. Hence $R(u) = R_1(u) \oplus R_2(u)$.

Alternatively you can find the irreducible representations via block diagonalization of the original representations. If we define the change of basis matrix $V = [v_1, v_{21}, v_{22}]$ and we perform the change of basis trasformation on the original representation matrices, we find :

$$P'_{R(\sigma_1)} = VP_{R(\sigma_1)}V^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{6}$$

$$\tag{7}$$

$$P'_{R(C_3)} = VP_{R(C_3)}V^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}. \tag{8}$$

5. Construct the character table of C_{3v} !

The trivial representation maps all group elements to the identity. We have seen the 2D representation in the first part of this exercise. We can compute the traces of the represenation in the different conjugacy classes and obtain : $Tr(R(e)) = 2, Tr(R(C_3)) = -1, Tr(R(\sigma_1)) = 0$. Now we can either identify another irreducible representation i.e. the anti-symmetric representation that maps cyclic permutation to 1 but transpositions to -1. Or we use the orthogonality of characters to fill the last row of the character table. For example we have :

Conjugacy Class	$\{e\}$	$\{(12),(13),(23)\}$	$\{(123),(132)\}$
Trivial Representation	1	1	1
Standard Representation	2	0	-1
Sign Representation	1	x	y

where the entry of 1 is known as $Tr(R(e)) = dim(R)$ and we know from Burnside's Lemma that $dim(R) = 1$. Then by orthogonality we have :

$$1 * 2 * 1 + 3 * 0 * x + 2 * (-1) * y = 0 \tag{9}$$

$$1 * 1 * 1 + 3 * 1 * x + 2 * 1 * y = 0 \tag{10}$$

(here the first number is the number of elements in the conjugacy class, the second number is the character of the known rep. and the third number is the character of the representation we are looking for. Solving for x, y in the above gives us $y = 1, x = -1$ and therefore :

Conjugacy Class	$\{e\}$	$\{(12),(13),(23)\}$	$\{(123),(132)\}$
Trivial Representation	1	1	1
Standard Representation	2	0	-1
Sign Representation	1	-1	1

Problem 2 : Lie-Algebras and Infinitesimal Generators

This problem is intended to get you familiar with the basics of Lie Algebras and help you understand the relationship between $SU(2)$ and $SO(3)$... which in turn will help you (hopefully!) have a better understanding of why the Bloch sphere representation of quantum states works.

1. Compute a 3D representation of the basis of the Lie-Algebra of SO(3). Then compute the structure constants (commutator) among the basis elements. Show that the representation $\rho : SO(3) \to GL(\mathbb{R}^3)$ with $\rho(A) = e^{a_i X_i}$, $A \in SO(3)$, $a_i \in \mathbb{R}$ representing the rotation (for example angles) and X_i the basis elements of so(3), is a valid representation of SO(3) (this is called the fundamental representation of SO(3)).
Hint : The Lie-Algebra is formally defined as the tangent space to the Lie-Group at the identity element. In practice we can use this to compute the Lie-Algebra by means of the exponential map. In fact any element $A \in G$ can be written as $A(t) = e^{tX}, X \in g$, where g is the Lie-Algebra. Therefore one can access elements by looking at : $\frac{d}{dt}A(t)|_{t=0} \in g$.

To compute the Lie Algebra of $SO(3) = \{A \in Mat^{3\times 3}(\mathbb{R}) | A^T A = I, \det(A) = 1\}$ we use the properties of elements of SO(3). Let $A \in SO(3)$ i.e. $A^T A = 1, \det(A) = 1$. Write $A = e^{tX}$. We have : $A^T A = e^{tX} e^{tX^T} = 1$. Taking the derivative of both sides and evaluating at $t = 0$ yields : $X^T = -X$. Next we have $\det(A) = \det\left(e^{tX}\right) = e^{Tr(tX)} = 1$. Again with the derivative evaluated at $t = 0$, we obtain $Tr(X) = 0$. Therefore the Lie Algebra $so(3)$ of SO(3) is given by traceless, skew-symmetric 3×3 matrices. A basis for those is given by :
$$E_1 = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, E_2 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, E_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}.$$
For the commutation relation one gets : $[E_i, E_j] = \epsilon_{ijk} E_k$ and the structure constants are therefore given by ϵ_{ijk}.
If you take the Lie-algebra as a real vector space, you cannot diagonalize it (as the matrices have imaginary eigenvalues). Therefore in quantum mechanics we consider the complexified version of the group i.e. $SO(3)_{\mathbb{C}} = iSO(3)$ and then changing into the basis in which E_1 is diagonal, yields :
$$L_1 = \begin{pmatrix} 0 & -i/\sqrt{2} & 0 \\ i/\sqrt{2} & 0 & -i/\sqrt{2} \\ 0 & i/\sqrt{2} & 0 \end{pmatrix}, L_2 = \begin{pmatrix} 0 & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 0 \end{pmatrix}, L_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$
which lead to the known commutation relation $[L_i, L_j] = i\epsilon_{ijk} L_k$.

To show that this is indeed a representation consider two elements $A, B \in SO(3)$. We have $\rho(A) = e^{a_i L_i}, \rho(B) = e^{b_j L_j}$. Let $AB = C$. Then $\rho(A)\rho(B) = e^{a_i L_i} e^{b_j L_j} = e^{a_i L_i + b_j L_j + \frac{1}{2} a_i b_j [L_i, L_j] + \ldots} = e^{c_k L_k} = \rho(C) = \rho(AB)$ (Baker-Campbell-Hausdorff-Formula). The product of the exponentials of two operators gives the exponential of the sum of the operators plus a series of their commutators. Since the commutator of two basis elements X_i, X_j will again produce a basis element $i\epsilon_{ijk} X_k$ the expression will again be the exponential of a linear combination of X_k with new coefficients c_k.

2. Do the same for SU(2).
We have $SU(2) = \{A \in Mat^{2\times 2}(\mathbb{C}) | A^\dagger A = I, \det(A) = 1\}$. Similar to before the constraint on the determinant leads to traceless basis states for the Lie Algebra su(2). Instead of skew symmetric matrices we now have $X^\dagger + X = 0, X^\dagger = -X$, which leads to matrices of the form $\begin{pmatrix} ia & b+id \\ -b+id & -ia \end{pmatrix}$.
One possible basis is :
$\sigma_1 = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \sigma_3 = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$. Again taking the complexified version of the group $SU(2)_\mathbb{C} = iSU(2)$ we find a basis that you know very well : the Pauli matrices $i\sigma_i$ with commutation relations $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$.

3. It can be shown that the finite dimensional, irreducible representations of $SO(3)$ all have odd dimensions. They can be constructed with the help of the well known ladder operators $L_\pm = L_x \pm iL_y$ where $L_{x,y,z}$ form a basis of $so(3)$. In the basis in which L_z is diagonal i.e. $\{|l,m\rangle\}, L_z |l,m\rangle = m |l,m\rangle$, it can be shown that $L_\pm |l,m\rangle = \sqrt{(l+1\pm m)(l \mp m)}\, |l, m\pm 1\rangle$. Use this to i) compute the 3D irreducible representation of $SO(3)$ and ii) the 5D irreducible representation of $SO(3)$.
Hint : Compute the matrix representation of the ladder operators $L_\pm$ in the basis $\{|l,m\rangle\}$ and construct $L_{x,y}$ from there. We start with the 3D representation. We know L_z is diagonal with eigenvalues $-1, 0, 1$ i.e.
$$L_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$
Now we compute the representations of the ladder operators $L_\pm$. $\sqrt{(l+1\pm m)(l\mp m)} = \sqrt{(2\pm m)(1\mp m)} = 0/\sqrt{2}, \sqrt{2}/\sqrt{2}, \sqrt{2}/0$ for $m = 1, 0, -1$ and L_+/L_-. Therefore :
$$L_\pm = \begin{pmatrix} \langle 1|L_\pm|1\rangle & \langle 1|L_\pm|0\rangle & \langle 1|L_\pm|-1\rangle \\ \langle 0|L_\pm|1\rangle & \langle 0|L_\pm|0\rangle & \langle 0|L_\pm|-1\rangle \\ \langle -1|L_\pm|1\rangle & \langle -1|L_\pm|0\rangle & \langle -1|L_\pm|-1\rangle \end{pmatrix} = \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \text{ or } \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$
for L_+ and L_-, respectively. We also have : $L_x = \frac{1}{2}(L_+ + L_-) = \begin{pmatrix} 0 & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 0 \end{pmatrix}$
and $L_x = \frac{-i}{2}(L_+ - L_-) = \begin{pmatrix} 0 & -i/\sqrt{2} & 0 \\ i/\sqrt{2} & 0 & -i/\sqrt{2} \\ 0 & i/\sqrt{2} & 0 \end{pmatrix}$.
The same procedure for 5D gives :
$$L_z = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -2 \end{pmatrix}, L_+ = \begin{pmatrix} 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{6} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{6} & 0 \\ 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \text{ and } L_- = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{6} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{6} & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \end{pmatrix}$$
Again with $L_x = \frac{1}{2}(L_+ + L_-)$,$L_y = \frac{-i}{2}(L_+ - L_-)$ we have :
$$L_x = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & \frac{\sqrt{3}}{\sqrt{2}} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{\sqrt{2}} & 0 & \frac{\sqrt{3}}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{\sqrt{2}} & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \text{ and } L_y = \begin{pmatrix} 0 & -i & 0 & 0 & 0 \\ i & 0 & \frac{-i\sqrt{3}}{\sqrt{2}} & 0 & 0 \\ 0 & \frac{i\sqrt{3}}{\sqrt{2}} & 0 & \frac{-i\sqrt{3}}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{i\sqrt{3}}{\sqrt{2}} & 0 & -i \\ 0 & 0 & 0 & i & 0 \end{pmatrix}$$

4. For SU(2) the irreducible representations can have any dimension and we have the same ladder operators as for SO(3). i) Compute the 2D irreducible representation of SU(2). ii) Compute the 3D irreducible representation of SU(2). Compare with the one from SO(3). For 2D we already know a representation, namely the Pauli matrices. For 3D we can follow the same logic as above and end up with exactly the same representation for SU(2) as for SO(3).
5. Is the 3D representation of SO(3) you have derived also a representation of SU(2) ? Explain why this makes sense with respect to the Bloch sphere.
   Yes it is. In fact any representation of SO(3) is also a representation of SU(2). The converse is not true. For example there is a 2D representation of SU(2) (spin-1/2) which is not a proper representation of SO(3). This is also visible in the possible dimensions : odd for SO(3) while arbitrary for SU(2). For each representation in SO(3) there are two in SU(2), and we talk about SU(2) being a double cover of SO(3). (Bonus - non examinable - are all representations of SU(2) also representations of SO(3) ? What about vice versa ?)