Quantum mechanics II, Problems 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 $\Psi_1(\mathbf{r}) = x^2 e^{-r}$, $\Psi_2(\mathbf{r}) = y^2 e^{-r}$, $\Psi_3(\mathbf{r}) = 2xye^{-r}$. 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.

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

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

   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 :

$$P_{R(u)} \Psi(\mathbf{r}) \equiv \Psi(R^{-1}(u)\mathbf{r}), \, \forall u \in C_{3v},$$

   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.

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

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

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

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 $\rho(A) = \mathrm{e}^{a_i X_i}$, $A \in SO(3)$, $a_i \in \mathbb{R}$ 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 $A(t) = \mathrm{e}^{tX}, X \in g$, where g is the Lie-Algebra. Therefore one can access elements by looking at : $\frac{d}{dt}A(t)|_{t=0} \in g$.
2. Do the same for SU(2).
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.
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).
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.

   (Bonus - non examinable - are all representations of SU(2) also representations of SO(3) ? What about vice versa ?)