Continuous Symmetries and Lie Algebras

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Abstract

Continuous symmetries are an important tool in the calculation of eigenstates of the Hamiltonian in quantum mechanics. With the example of the hydrogen atom, we show how Lie groups and Lie algebras are used to represent symmetries in physics and how Lie group and Lie algebra representations are defined and calculated. In addition to the rotational symmetry of the hydrogen atom, the Runge-Lenz vector is also considered to derive an $\mathfrak{so}(4)$ symmetry. Finally, using this symmetry the energy eigenvalues $E_n = -\frac{mk^2}{2n^2}$ with their their n^2 degeneracy are calculated.

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1 Introduction and Motivation

In previous talks we have seen that symmetries can be used to simplify the calculation of eigenstates of the Hamiltonian. More precisely, we observed representations of the finite groups describing the symmetries. Using the fact, that the symmetries commute with the Hamiltonian it suffices to calculate the Eigenstates of the group representation. But so far we have only seen discrete symmetries (thus finite groups). In this part of the seminar we analyse how we can use similar methods for continuous symmetries, more precisely we investigate representations of Lie groups and their respective Lie algebras.

This report is organized as follows. We begin by introducing the hydrogen atom as the main example of the theories discussed and a classical motivation using Noether's theorem. In section 2 the mathematical foundation needed to calculate irreducible representations is covered by a discussion on Lie groups and algebras. Knowing about the mathematical tools we immerse ourselves into the rotational symmetry of the Hydrogen atom and calculate the eigenstates of the Hamiltonian. Finally, in section 4 the Runge-Lenz vector is introduced to investigate the $\mathfrak{so}(4)$ symmetry of the problem, which enables the calculation of the energy eigenvalues and their degeneracy.

1.1 Hydrogen Atom

During the derivations to come we will repeatedly come back to one specific example: The hydrogen atom. First, we will analyse the spherical symmetry of the Coulomb potential to derive the eigenstates of the Hamiltonian:

$$\mathsf{H} = \frac{\mathsf{p}^2}{2\mathsf{m}} - \frac{\mathsf{k}}{\mathsf{r}}, \quad \mathsf{k} = \mathsf{e}^2 \tag{1}$$

Later however, we will observe that there is another hidden symmetry to this problem which will allow further investigation into the energy eigenstates of the hydrogen atom.

1.2 Continuous Symmetries and Noether's Theorem

Even though finite dimensional groups are certainly easier to understand than the groups describing continuous symmetries, the latter also have properties we can use that are not available in the finite case. In particular, we know from classical mechanics that we can use Noether's theorem to connect continuous symmetries to conserved quantities.[5]

Theorem 1.1. *(Noether) Assume we have a system described by generalized coordinates $q_1, \dots, q_n$ and the Lagrangian $\mathcal{L}(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n, t)$. Further assume that an infinitesimal transformation*

$$q_i(t) \mapsto q_i(t) + \delta q_i(t) \tag{2}$$

is a symmetry transformation, i.e. the action is invariant under this transformation. Then there is a conserved quantity of the system

$$J = \sum_i \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \delta q_i - F \tag{3}$$

where $\frac{dF}{dt} = \Delta\mathcal{L}$ *is the change to the Lagrangian under the transformation.*

As a first example we analyse the rotational symmetry of the hydrogen atom (equation 1). As Noether's theorem is stated in the Lagrangian formalism, we have to perform a Legendre transform to derive the Lagrangian.

$$\mathcal{L} = \frac{1}{2} m\dot{q}^2 + \frac{k}{|q|}, \quad q = (x, y, z)^T \tag{4}$$

To find the constant of motion corresponding to the symmetry we look at infinitesimal transformations, e.g. we start with an infinitesimal rotation ($\phi \to 0$) around the x-axis:

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\phi) & -\sin(\phi) \\ 0 & \sin(\phi) & \cos(\phi) \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \approx \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \tag{5}$$

where we performed a first order Taylor approximation around $\phi = 0$. This now allows to write the transformation in the form of the theorem:

$$\begin{aligned} x &\mapsto x + \delta x = x + 0 \\ y &\mapsto y + \delta y = y - z \\ z &\mapsto z + \delta z = z + y \end{aligned}$$

Note that in this case not only the action, but also the Lagrangian is invariant under the transformation, thus, $\Delta\mathcal{L} = 0$. The conserved quantity is then given as

$$\frac{\partial \mathcal{L}}{\partial \dot{x}} \delta x + \frac{\partial \mathcal{L}}{\partial \dot{y}} \delta y + \frac{\partial \mathcal{L}}{\partial \dot{z}} \delta z = 0 - m\dot{y}z + m\dot{z}y = L_x \tag{6}$$

the x component of the angular momentum. Similarly, using rotations around the y and z axis, we find that L_y and L_z are conserved.

2 Lie Groups and Lie Algebras

As we have seen in the example above, the rotational symmetry (for example in the hydrogen atom) is mathematically described through the special orthogonal group $SO(3)$. It turns out that $SO(3)$ – like all groups describing a continuous symmetry – is a Lie group. It, thus, certainly make sense to look at the mathematical definition.

Definition 2.1. *A* ***Lie group*** *is a set endowed simultaneously with the compatible structures of a group and a $\mathcal{C}^\infty$ manifold. Meaning that the multiplication and inverse operations in the group structure are differentiable maps.[1]*

The most common example for a Lie group is the general linear group $GL(n)$. Many other Lie groups can be defined as subgroups of $GL(n)$, such as the (special) orthogonal groups $O(n)$, $SO(n)$, the symplectic group $Sp(n)$ or the special linear group $Sl(n)$. Although, of course, not all Lie algebras are subgroups of $GL(n)$, we will in the following sections restrict ourselves to matrix Lie groups, in order to simplify some of the discussions significantly.

Now that we know the mathematical construct which describes the symmetry, we would like to know how Lie group representations are defined. In fact, the definition is identical to the case of finite groups.

Definition 2.2. *A* ***representation*** $\rho : G \to GL(V)$ *of a Lie group G is a morphism from G to the group of automorphisms on a vector space V. Meaning for $g, h \in G$, $v \in V$ it holds that $\rho(g \cdot h)v = \rho(g) \circ \rho(h)v$.*

Sadly, the methods we used for finite groups, such as finding a character table to derive the irreducible representations, no longer work in the case of Lie groups as they have an infinite number of elements.

An interesting fact, however, is that if G is a connected Lie group, any neighbourhood $U \subset G$ of the identity generates G. This means that a representation $\rho : G \to H$ is uniquely determined by what it does on any open set containing the identity in G. More precisely, it can be shown that ρ is uniquely determined by its differential at the identity $d\rho_e$. How exactly this can be done, will now be investigated. [1]

2.1 Lie Algebras

As of the last comment in the previous subsection it seems to make sense to have a closer look at the tangent space T_eG of G at the identity. Especially, we would like to know which maps $\sigma : T_eG \to T_eH$ on the tangent space of G are differentials of a representation $\rho : G \to H$. [1]

Theorem 2.1. *Let G and H be matrix Lie groups with G simply connected and let $\mathfrak{g} = T_eG$ and $\mathfrak{h} = T_eH$ be their respective tangent spaces at the identity. A linear map $\sigma : \mathfrak{g} \to \mathfrak{h}$ is the differential of a map $\rho : G \to H$, if and only if σ preserves the commutator, meaning for $x, y \in \mathfrak{g}$*

$$[\sigma(x), \sigma(y)] = \sigma([x, y]), \tag{7}$$

where $[x, y] = xy - yx$.

The proof to this theorem can be found in [1]. This proposition motivates the following definition.

Definition 2.3. *A **Lie algebra** $\mathfrak{g}$ is a vector space together with a bilinear map*

$$[,] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g} \tag{8}$$

called the Lie bracket, such that $\forall x, y \in \mathfrak{g}$ the properties

- $[x, y] = -[y, x]$ *(skew symmetric)*
- $[x, [y, z]] + [y, [z, x]] + [z, [x, y]] = 0$ *(Jacobi identity)*

are fulfilled.

In particular, for a matrix Lie group G we can define its Lie algebra $\mathfrak{g} = T_eG$ as the tangent space at the identity with the commutator as the Lie bracket. Again motivated by proposition 2.1 we define representations of Lie algebras.

Definition 2.4. *A **Lie algebra representation** is a linear map $\rho : \mathfrak{g} \to \mathfrak{gl}(V)$ from the Lie algebra $\mathfrak{g}$ to the vector space $\mathfrak{gl}(V) = M_{n\times n}$ of endomorphisms of a vector space V, that preserves the Lie bracket.*

How does this simplify the procedure of finding irreducible representations, you might ask? The beauty of the Lie algebra is, that we now work with a (most likely finite dimensional) vector space instead of the infinite group. Thus, it suffices to find out how the basis elements of this vector space are represented. Instead of observing an infinite number of group elements we only need to understand what the representation does with a few elements in a vector space.

[1] Another motivation originates from Noether's theorem: In the example discussed above we used the Taylor approximation of an infinitesimal rotation to describe the transformation, i.e. we linearised the transformation. This is essentially the same idea as looking at the tangent space at the identity of the Lie group.

2.2 The Exponential Map

In this subsection we analyse how we can use the exponential map to transform a representation of the Lie algebra back to its corresponding Lie group representation. Again we restrict ourselves to matrix Lie groups.

Definition 2.5. *The **exponential map*** $\exp : \mathfrak{g} \to G$ *for a matrix Lie group* G *and its corresponding Lie algebra* $\mathfrak{g}$ *is defined as*

$$\exp(x) = \sum_{k=0}^{\infty} \frac{x^k}{k!} \tag{9}$$

Of course we need to prove that this definition is indeed well defined. We show this for the case that the matrix Lie group is closed.

Proof. Let $x \in \mathfrak{g} = T_e G$ such that $X(t) \in G$ is the curve with $X(0) = e$ and $\frac{d}{dt}X(t)\big|_{t=0} = x$. Let $t \in \mathbb{R}$ and define the sequence $X_n = X(\frac{t}{n})^n \in G$. We find

$$\begin{aligned} \lim_{n\to\infty} X_n = \lim_{n\to\infty} X\left(\frac{t}{n}\right)^n &\overset{Taylor}{=} \lim_{n\to\infty} \left(e + \frac{t}{n}x + \mathcal{O}\left(\frac{1}{n^2}\right)\right)^n \\ &= \lim_{n\to\infty} \exp\left(\frac{t}{n}x + \mathcal{O}\left(\frac{1}{n^2}\right)\right)^n \\ &= \lim_{n\to\infty} \exp\left(tx + \mathcal{O}\left(\frac{1}{n}\right)\right) \\ &= \exp(tx) \end{aligned}$$

As we assumed G to be closed, the limit of the sequence X_n is contained in G and, thus, for $t = 1$ we find that indeed $\exp(x) \in G$. □

So apparently we can use the exponential to map elements of the Lie algebra into the Lie group. Even better news is that this works similarly for representations: [2]

Theorem 2.2. *Let* G *be a matrix Lie group with Lie algebra* $\mathfrak{g}$ *and let* $\rho : G \to GL(V)$ *be a finite dimensional representation of* G*. Then there is a unique representation* $\sigma : \mathfrak{g} \to \mathfrak{gl}(V)$*, such that*

$$\rho(\exp(x)) = \exp(\sigma(x)) \tag{10}$$

for all $x \in \mathfrak{g}$*. The representation* σ *can be computed as*

$$\sigma(x) = \frac{d}{dt}\left[\rho(\exp(tx))\right]\Big|_{t=0} \tag{11}$$

If G is additionally simply connected, we can even state the following proposition:

Theorem 2.3. *Let* $\mathfrak{g}$ *be the corresponding Lie algebra of a simply connected Lie group* G *and let* $\sigma : \mathfrak{g} \to \mathfrak{gl}(V)$ *be a representation of* $\mathfrak{g}$ *on* V*. Then there is a corresponding representation* $\rho : G \to GL(V)$ *of the Lie group, uniquely determined by the condition*

$$\sigma(x) = \frac{d}{dt}\left[\rho(\exp(tx))\right]\Big|_{t=0} \tag{12}$$

3 Representation Theory of $\mathfrak{sl}(2, \mathbb{C})$

3.1 Lie Algebra of $SO(3)$

Our goal is to use the theory discussed above to determine the eigenstates of the hydrogen atom. Thus, we are interested in the Lie algebra of the group of rotations $SO(3)$. To find the tangent space at the identity we observe rotations around the three principal axes:

$$R_x(\phi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\phi) & -\sin(\phi) \\ 0 & \sin(\phi) & \cos(\phi) \end{pmatrix}, R_y(\theta) = \begin{pmatrix} \cos(\theta) & 0 & \sin(\theta) \\ 0 & 1 & 0 \\ -\sin(\theta) & 0 & \cos(\theta) \end{pmatrix}, R_z(\psi) = \begin{pmatrix} \cos(\psi) & -\sin(\psi) & 0 \\ \sin(\psi) & \cos(\psi) & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{13}$$

Those generate the Lie group and it, thus, suffices to derive the three principal rotations to find a basis (the generators) for the tangent space, i.e. the Lie algebra. We find

$$L_x = \frac{d}{d\phi} R_x(\phi)\big|_{\phi=0} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$L_y = \frac{d}{d\theta} R_y(\theta)\big|_{\theta=0} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}$$

$$L_z = \frac{d}{d\psi} R_z(\psi)\big|_{\psi=0} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Note that using the exponential map defined above, we can map the generators back onto their rotational matrices, e.g. $\exp(\phi L_x) = R_x(\phi)$. The Lie brackets of this Lie algebra are well known:

$$[L_i, L_j] = \varepsilon_{ijk} L_k \tag{14}$$

To find the irreducible representations of $\mathfrak{so}(3)$ we need another trick, which will be shown in the next subsection.

Important: The definition of the above generators is the mathematical convention. In physics, the generators are multiplied with the imaginary unit $\mathsf{L_i} = iL_i$, which leads to the commutation relations known from quantum mechanics:

$$[\mathsf{L_i}, \mathsf{L_j}] = i\varepsilon_{ijk} \mathsf{L_k} \tag{15}$$

In the following we will use the mathematical convention in the theoretical derivations but switch to the physical convention when talking about the operators in the Hilbert space. To avoid confusion, generators in physical convention will be displayed in sans serif font.

3.2 Isomorphism $\mathfrak{so}(3) \otimes \mathbb{C} \to \mathfrak{sl}(2, \mathbb{C})$

The problem with $\mathfrak{so}(3)$ is, that none of the generators are diagonal. As we will see later, finding the irreducible representations is a much simpler task, if we have at least one diagonal basis element. Luckily, we can show that $\mathfrak{so}(3)$ is, after complexification, isomorphic to the Lie algebra of the special linear group $\mathfrak{sl}(2, \mathbb{C})$, where this condition is fulfilled.

The Lie algebra $\mathfrak{sl}(2, \mathbb{C})$ is given as the vector space of traceless 2×2 matrices.[2] A natural basis is

$$h = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad e = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad f = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \tag{16}$$

which has the commutation relations

$$[h, e] = 2e, \quad [h, f] = -2f, \quad [e, f] = h \tag{17}$$

We can now define the linear map $\Psi : \mathfrak{so}(3) \otimes \mathbb{C} \to \mathfrak{sl}(2, \mathbb{C})$ by

$$L_x \mapsto \frac{1}{2}(e - f), \quad L_y \mapsto \frac{i}{2}(e + f), L_z \mapsto \frac{i}{2}h, \tag{18}$$

By definition, Ψ is bijective. It remains to be shown that Ψ preserves the Lie bracket:

$$\begin{aligned}
[\Psi(L_x), \Psi(L_y)] &= \frac{i}{4}[e - f, e + f] = \frac{i}{4}\big([e, f] - [f, e]\big) = \frac{i}{4}(2h) = L_z = [L_x, L_y] \\
[\Psi(L_y), \Psi(L_z)] &= -\frac{1}{4}[e + f, h] = -\frac{1}{4}\big([e, h] + [f, h]\big) = \frac{1}{4}(2e - 2f) = L_x = [L_y, L_z] \\
[\Psi(L_z), \Psi(L_x)] &= \frac{i}{4}[h, e - f] = \frac{i}{4}\big([h, e] - [h, f]\big) = \frac{i}{4}(2e + 2f) = L_y = [L_z, L_x]
\end{aligned}$$

So indeed, Ψ is an isomorphism of Lie algebras and from now on we can work with $\mathfrak{sl}(2, \mathbb{C})$ instead of $\mathfrak{so}(3)$. Once we have found a representation $\sigma : \mathfrak{sl}(2, \mathbb{C}) \to \mathfrak{gl}(V)$, we can define $\rho = \Psi^{-1} \circ \sigma : \mathfrak{so}(3) \otimes \mathbb{C} \to \mathfrak{gl}(V)$ to find a representation on $\mathfrak{so}(3)$.

[2] We will not use the connection to the Lie group $SL(2, \mathbb{C})$, thus this derivation is omitted. It suffices at the moment to think of $\mathfrak{sl}(2, \mathbb{C})$ as this vector space together with the commutator as Lie bracket.

3.3 Simple Lie Algebras

Before we start determining the irreducible representations of $\mathfrak{sl}(2,\mathbb{C})$, we need some more definitions and results from Lie algebra representation theory.[1]

Definition 3.1. *A Lie subalgebra $\mathfrak{h} \subset \mathfrak{g}$ is called ideal, if $[\mathfrak{h},\mathfrak{g}] \subset \mathfrak{h}$.*

Definition 3.2. *A Lie algebra $\mathfrak{g}$ is called **simple**, if it has no non-trivial ideals.*

Simple[3] Lie algebras have some useful properties:

Theorem 3.1 (Complete Reducibility)**.** *Let V be a representation of the simple Lie algebra $\mathfrak{g}$ and $W \subset V$ a subspace invariant under the action of $\mathfrak{g}$. then there exists another invariant subspace $W' \subset V$ such that $V = W \oplus W'$. Thus, V is completely reducible.*

This proposition is crucial, as it allows the decomposition in irreducible representations as we know it from finite groups. It also insures us that it suffices to look at the irreducible representations.

Theorem 3.2 (Preservation of Jordan Decomposition)**.** *Let $\mathfrak{g}$ be a simple matrix Lie algebra and $x \in \mathfrak{g}$, let $\rho : \mathfrak{g} \to \mathfrak{gl}(V)$ be a representation. Then ρ preserves the Jordan decomposition $x = D + N$ (where D is diagonal and N nilpotent), i.e.*

$$\rho(x) = \rho(D) + \rho(N), \tag{19}$$

where $\rho(D)$ is diagonal and $\rho(N)$ nilpotent.

An important consequence of this proposition is that, if $x \in \mathfrak{g}$ is diagonal, then for any representation $\rho : \mathfrak{g} \to \mathfrak{gl}(V)$ the action $\rho(x)$ is diagonal as well. After this discussion, we of course hope that the Lie algebra in question ($\mathfrak{sl}(2,\mathbb{C})$) is a simple Lie algebra. Luckily, the answer is yes.

Proof. Assume $\mathfrak{sl}(2,\mathbb{C})$ was not simple. Then there exists a non-trivial ideal $\mathfrak{h} \subset \mathfrak{sl}(2,\mathbb{C})$. As $\mathfrak{h}$ is non-trivial, it is at least one dimensional and contains a basis element $x = \alpha h + \beta e + \gamma f$, where h, e, f is the basis defined above. Since $\mathfrak{h}$ is ideal, $[h, x]$ is contained in $\mathfrak{h}$. We calculate

$$[h, x] = \alpha[h, h] + \beta[h, e] + \gamma[h, f] = 2e\beta - 2f\gamma \in \mathfrak{h}. \tag{20}$$

Thus, either $\alpha = 0$ or $h \in \mathfrak{h}$. If the latter was true, then $[h, e] = 2e \in \mathfrak{h}$ and $[h, f] = -2f \in \mathfrak{h}$, hence, $\mathfrak{h} = \mathfrak{sl}(2,\mathbb{C})$, contradicting the assumption. If, however, $\alpha = 0$ we find

$$[e, x] = \beta[e, e] + \gamma[e, f] = \gamma h \in \mathfrak{h}. \tag{21}$$

As shown above, $h \notin \mathfrak{h}$, thus $\gamma = 0$. Similarly we can show $\beta = 0$, thus $\mathfrak{h}$ is trivial and $\mathfrak{sl}(2,\mathbb{C})$ is simple. □

[3] In fact, the following theorems are also valid for semisimple Lie algebras. See [1]

3.4 Irreducible Representations of $\mathfrak{sl}(2,\mathbb{C})$

Finally, we have done the ground work to now construct the irreducible representations. Let $\rho : \mathfrak{sl}(2,\mathbb{C}) \to \mathfrak{gl}(V)$ be an irreducible finite-dimensional representation of $\mathfrak{sl}(2,\mathbb{C})$. Due to proposition 3.2, we know that for the canonical basis $\{h, e, f\}$ defined above $\rho(h)$ is diagonal and we can decompose the vector space V into eigenspaces V_α of $\rho(h)$:

$$V = \bigoplus_\alpha V_\alpha \tag{22}$$

meaning that for any $v \in V_\alpha$ we have $\rho(h)v = \alpha v$. In a next step we need to find out how e and f act on the eigenspaces V_α. To do this we observe

$$\rho(h)\rho(e)v = [\rho(h), \rho(e)]v + \rho(e)\rho(h)v = 2\rho(e)v + \alpha\rho(e)v = (2 + \alpha)\rho(e)v \tag{23}$$

and see that $\rho(e) : V_\alpha \to V_{\alpha+2}$ increases the eigenvalue (of v under the action of h) by 2. Similarly we can show that $\rho(f)$ decreases the eigenvalue by 2. By assumption V is finite-dimensional, thus for some α the eigenspace $V_\alpha = 0$ has to be trivial. We denote V_n as the last non-trivial eigenspace, i.e. $V_{n+2} = 0$.

We now claim that acting with f on $v \in V_n$ inductively spans the whole vector space, meaning $span\{v, \rho(f)v, \rho(f)^2v, \dots\} = V$.

Proof. As per assumption V is irreducible, it suffices to show that $W = span\{v, \rho(f)v, \rho(f)^2v, \dots\}$ is invariant under the action of ρ. Obviously, W is invariant under $\rho(f)$. As all $\rho(f)^kv \in V_{n-2k}$ are eigenvectors of $\rho(h)$, W is also invariant under $\rho(h)$. It remains to be shown that $\rho(e)W \subset W$. We know $\rho(e)v = 0$ as $v \in V_n$, next we check

$$\rho(e)\rho(f)v = [\rho(e), \rho(f)]v + \rho(f)\rho(e)v = \rho(h)v = nv \in W \tag{24}$$

also for the next element

$$\begin{aligned}\rho(e)\rho(f)^2v =& [\rho(e), \rho(f)]\rho(f)v + \rho(f)\rho(e)\rho(f)v = \\ & \rho(h)\rho(f)v + n\rho(f)v = (n-2)\rho(f)v + n\rho(f)v \in W.\end{aligned}$$

Similarly, one can show by induction that $\rho(e)\rho(f)^kv = k(n - k + 1)\rho(f)^{k-1}v \in W$ and, thus, $W = V$. □

We now again address the finite-dimensionality of V: In addition to the upper bound V_n there is also an k such that $\rho(f)^kv = 0$ for $v \in V_n$, representing a lower bound. We set m to be the smallest number that satisfies this condition, i.e. $\rho(f)^{m-1}v \neq 0$. If we look at the formula derived above we find

$$0 = \rho(e)\rho(f)^mv = m(n - m + 1)\rho(e)^{m-1}v. \tag{25}$$

Because we chose m such that $\rho(f)^{m-1}v \neq 0$, we now know that $n = m - 1 \in \mathbb{N}_0$ must be a non-negative integer. [1]

To summarise: The irreducible representations of $\mathfrak{sl}(2, \mathbb{C})$ are given by the $n+1$-dimensional vector spaces $V^n = span\{v, \rho(f)v, \rho(f)^2 v, \ldots, \rho(f)^n v\}$, where v is an eigenvector of $\rho(h)$ with eigenvalue n, such that $\rho(e)v = 0$. Applying $\rho(f)$ to v reduces the eigenvalue by 2 until $\rho(f)^n v$ has an eigenvalue of $-n$ and $\rho(f)^{n+1} = 0$.

3.5 Representations of $SO(3)$

Finally, we aim to lift the Lie algebra representations of $\mathfrak{so}(3)$ derived above to their corresponding Lie group representations. There is one problem, however: $SO(3)$ is not simply connected and, thus, proposition 2.3 cannot be applied in this case. So our goal is to find out, which irreducible representations V^n are representations of $SO(3)$. [2]

From quantum mechanics we know that the orbital angular momentum operator $\mathsf{L_z}$ only has integer eigenvalues. If we naively connect the operator with the $\mathfrak{so}(3)$ generator L_z we see that it is proportional to $h/2$ (equation 18). But in the previous subsection we found out that for the irreducible representation V^n, h has eigenvalues $\lambda_k = (n - 2k)$ for $n \in \mathbb{N}_0, k \in 0, \ldots, n$. If we want the eigenvalues of $\mathsf{L_z} \cong \frac{h}{2}$ to be integer, λ_k need to be even and, thus, n needs to be even. From this discussion we suspect that only the even representations V^{2n} of $\mathfrak{sl}(2, \mathbb{C})$ are representations of $SO(3)$.

Theorem 3.3. *Let $\sigma_n : \mathfrak{so}(3) \to \mathfrak{gl}(V^n)$ be an irreducible representation as in the previous subsection. If n is even, there exists a representation $\rho_n : SO(3) \to GL(V^n)$ such that $\rho_n(\exp(x)) = \exp(\sigma_n(x))$. If n is odd, this representation does not exist.*

Proof. Suppose n is odd and ρ_n existed. First, note that $\exp(2\pi L_z) = id_G$. Thus, we find

$$\rho_n(\exp(2\pi L_z)) = \rho_n(id_G) = \mathbb{I}_V \tag{26}$$

If we, however, first calculate the action of L_z in V^n, we find (in the canonical basis $\{v, \sigma_n(f)v, \ldots, \sigma_n(f)^n v\}$ of eigenvectors of $\sigma_n(h)$):

$$\sigma_n(L_z) = \frac{i}{2} \begin{pmatrix} \frac{i}{2}n & & & \\ & \frac{i}{2}(n-2) & & \\ & & \ddots & \\ & & & -\frac{i}{2}n \end{pmatrix} \tag{27}$$

Due to proposition 2.2 we now know that

$$\rho_n(\exp(2\pi L_z)) = \exp(2\pi\sigma_n(L_z)) = \begin{pmatrix} \exp(i\pi n) & & & \\ & \exp(i\pi(n-2)) & & \\ & & \ddots & \\ & & & \exp(-i\pi n) \end{pmatrix} = -\mathbb{I}_V, \tag{28}$$

contradicting the first calculation. Thus, ρ_n cannot exist.
The proof that the even representations exist is based on the fact, that the above contradiction does not exist for even n. A rigorous proof can be found in [2]. □

The proposition, thus, legitimates the thought at the beginning of this subsection. To bring it all together, we will look at how we connect the irreducible representations V^n with the known eigenstates of the hydrogen atom $|l, m\rangle$:

- The irreducible representation $V^{n=2l}$ corresponds to the eigenspace $\mathcal{H}_l$ of the total orbital angular momentum L^2. It has dimension $2l + 1$.
- The eigenvalues of the $\mathsf{L_z}$ operator are $\frac{n}{2}, \frac{n-2}{2}, \ldots, \frac{-n}{2} \approx l, l-1, \ldots, -l$ and correspond to the quantum number m.
- While e and f are used to raise and lower the eigenvalues of h in $\mathfrak{sl}(2, \mathbb{C})$, $\mathsf{L}_+ \cong e$ and $\mathsf{L}_- \cong f$ are the raising and lowering operators in the Hilbert space.

4 Runge-Lenz Vector

So far we used the rotational $SO(3)$ symmetry of the hydrogen atom to find the eigenstates of the Hamiltonian using representation theory. Further, using Noether's theorem we found the conserved quantity corresponding to the symmetry: The orbital angular momentum. But even though it seems as we have solved the hydrogen atom, there is more to be found in its symmetries. From classical mechanics we know that in a central potential $V(r) = \frac{k}{r}$ (known as the Kepler problem) the Runge-Lenz vector

$$\vec{M} = \vec{v} \times \vec{L} - k\frac{\vec{r}}{r} \tag{29}$$

is another constant of motion. This history of this vector is quite interesting, as it was (re-)discovered by many physicists over the years, due to its physical meaning being somewhat unintuitive compared to the angular momentum. In fact, the physical meaning lies in the fact that

$$\vec{L} \cdot \vec{M} = 0 \tag{30}$$

it is orthogonal to the angular momentum. This of course means that the direction of $\vec{M}$ always points into the plane of the orbit. Additionally, if we look at the magnitude

$$|\vec{M}| \propto \varepsilon \tag{31}$$

we find that it describes the eccentricity of the orbit in the Kepler problem. [6]

The hope is of course, that we can find a correspondence to the classical Runge-Lenz vector in the quantum mechanical hydrogen atom. Indeed, this can be done: To find the corresponding operator we simply take the hermitian part of the classical vector and apply the correspondence principle:

$$\mathsf{M} = \frac{1}{2\mathsf{m}}\mathsf{p} \times \mathsf{L} - \frac{1}{2\mathsf{m}}\mathsf{L} \times \mathsf{p} - \mathsf{k}\frac{\mathsf{r}}{|\mathsf{r}|} \tag{32}$$

To check that M is a constant of motion we compute the commutator with the Hamiltonian and find that indeed

$$[\mathsf{H}, \mathsf{M_i}] = 0 \tag{33}$$

Thus, Noether's theorem states that there has to be an underlying continuous symmetry corresponding to this conserved quantity.

4.1 $\mathfrak{so}(4)$ Symmetry of the Hydrogen Atom

To find the Lie algebra corresponding to the Runge-Lenz vector, we compute some more commutators:

$$[\mathsf{L_i}, \mathsf{M_j}] = i\varepsilon_{ijk}\mathsf{M_k}$$
$$[\mathsf{M_i}, \mathsf{M_j}] = -i\varepsilon_{ijk}\mathsf{L_k}(2/\mathsf{m})\mathsf{H}$$

The second relation motivates to a redefinition of M in the eigenspace of H with energy $E < 0$ as

$$\tilde{\mathsf{M}}_\mathsf{i} = \sqrt{\frac{\mathsf{m}}{-2\mathsf{E}}}\mathsf{M_i}, \tag{34}$$

leading to the much simpler relation $[\tilde{\mathsf{M}}_\mathsf{i}, \tilde{\mathsf{M}}_\mathsf{j}] = i\varepsilon_{ijk}\mathsf{L_k}$. Together with $[\mathsf{L_i}, \mathsf{L_j}] = i\varepsilon_{ijk}\mathsf{L_k}$ those are, as we will show, exactly the commutation relations of the Lie algebra $\mathfrak{so}(4)$.[4]

The generators of $\mathfrak{so}(4)$ can be found similarly to those of $\mathfrak{so}(3)$, they are

$$A_1 = \begin{pmatrix} 0 & \cdots \\ \vdots & L_x \end{pmatrix}, \quad A_2 = \begin{pmatrix} 0 & \cdots \\ \vdots & L_y \end{pmatrix}, \quad A_3 = \begin{pmatrix} 0 & \cdots \\ \vdots & L_z \end{pmatrix},$$

$$B_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & & \\ 0 & & \ddots & \\ 0 & & & 0 \end{pmatrix}, \quad B_2 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & & \\ -1 & & \ddots & \\ 0 & & & 0 \end{pmatrix}, \quad B_3 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & & \\ 0 & & \ddots & \\ -1 & & & 0 \end{pmatrix}$$

and have the commutation relations $[A_i, A_j] = \varepsilon_{ijk}A_k$, $[B_i, B_j] = \varepsilon_{ijk}A_k$ and $[A_i, B_j] = \varepsilon_{ijk}B_k$. Identifying A_i with the orbital angular momentum $\mathsf{L_i}$ and B_i with the Runge-Lenz vector in the energy eigenspace $\tilde{\mathsf{M}}_\mathsf{i}$[4] proofs the claim, that the hydrogen atom has an $\mathfrak{so}(4)$ symmetry. The question which we will have to answer next is what the irreducible representations of this Lie algebra are.

4.2 Isomorphism $\mathfrak{so}(4) \to \mathfrak{so}(3) \oplus \mathfrak{so}(3)$

To find the irreducible representations of $\mathfrak{so}(3)$ we used the isomorphism to $\mathfrak{sl}(2, \mathbb{C})$ which simplified this process dramatically. Sadly, there is no isomorphism from $\mathfrak{so}(4)$ to $\mathfrak{sl}(3, \mathbb{C})$ or a similar Lie algebra. However, we can still use the theory derived above in an even simpler way. To do this we transform the canonical basis $\{A_1, A_2, A_3, B_1, B_2, B_3\}$ of $\mathfrak{so}(4)$ into a new basis as follows:

$$X_i = \frac{1}{2}(A_i + B_i), \quad i \in \{1, 2, 3\}$$
$$Y_i = \frac{1}{2}(A_i - B_i), \quad i \in \{1, 2, 3\}$$

If we compute the commutators we find that

$$[X_i, Y_j] = \frac{1}{4}\big([A_i, A_j] - [A_i, B_j] + [B_i, A_j] - [B_i, B_j]\big) = \frac{1}{4}\varepsilon_{ijk}(A_k - B_k + B_k - A_k) = 0$$
$$[X_i, X_j] = \frac{1}{4}\big([A_i, A_j] + [A_i, B_j] + [B_i, A_j] + [B_i, B_j]\big) = \frac{1}{4}\varepsilon_{ijk}(A_k + B_k + B_k + A_k) = \varepsilon_{ijk}X_k$$
$$[X_i, X_j] = \frac{1}{4}\big([A_i, A_j] - [A_i, B_j] - [B_i, A_j] + [B_i, B_j]\big) = \frac{1}{4}\varepsilon_{ijk}(A_k - B_k - B_k + A_k) = \varepsilon_{ijk}Y_k.$$

We have, thus, split the $\mathfrak{so}(4)$ Lie algebra into two copies of $\mathfrak{so}(3)$ algebras, showing that $\mathfrak{so}(4) \cong \mathfrak{so}(3) \oplus \mathfrak{so}(3)$ are isomorph to each other!

To find the representations of $\mathfrak{so}(4)$ we can simply add up any two representations of $\mathfrak{so}(3)$.

[4]For this identification we have to keep in mind that the convention changes, thus $\mathsf{L}_\mathsf{i} \cong iA_i$ and $\tilde{\mathsf{M}}_\mathsf{i} \cong iB_i$.

4.3 Calculating the Energy Eigenvalues

Finally, we want to determine the energy eigenstates of the Hamiltonian H. To do this we state some further relations:

$$\mathsf{M} \cdot \mathsf{L} = \mathsf{L} \cdot \mathsf{M} = 0, \quad \mathsf{M}^2 = 2\mathsf{H}(\mathsf{L}^2 + 1)/\mathsf{m} + \mathsf{k}^2 \tag{35}$$

In the eigenspace of energy $E < 0$ we identify the Hamiltonian with the energy eigenvalue and solve for E:

$$\mathsf{E} = -\frac{\mathsf{mk}^2}{2(\tilde{\mathsf{M}}^2 + \mathsf{L}^2 + 1)} = -\frac{\mathsf{mk}^2}{2((\mathsf{X} - \mathsf{Y})^2 + (\mathsf{X} + \mathsf{Y})^2 + 1)} = -\frac{\mathsf{mk}^2}{2(2\mathsf{X}^2 + 2\mathsf{Y}^2 + 1)} \tag{36}$$

We know that the operators X and Y each span an $\mathfrak{so}(3)$ algebra. As they commute with the Hamiltonian, the eigenstates of H are also eigenstates of X and Y and we can, thus, use $\mathfrak{so}(3)$ representation theory which tell us that

$$\mathsf{X}^2 = \mathsf{j_x}(\mathsf{j_x} + 1), \quad \mathsf{Y}^2 = \mathsf{j_y}(\mathsf{j_y} + 1), \tag{37}$$

where j_x, j_y are integer or half-integer numbers. However, condition 35 tells us, that

$$0 = \tilde{\mathsf{M}} \cdot \mathsf{L} = (\mathsf{X} + \mathsf{Y}) \cdot (\mathsf{X} - \mathsf{Y}) = \mathsf{X}^2 - \mathsf{Y}^2 \implies \mathsf{X}^2 = \mathsf{Y}^2 \implies \mathsf{j_x} = \mathsf{j_y} = \mathsf{j} \tag{38}$$

the quantum numbers are equal for both copies of $\mathfrak{so}(3)$, leading to

$$\mathsf{E_n} = -\frac{\mathsf{mk}^2}{2(4\mathsf{j}(\mathsf{j} + 1) + 1)} = -\frac{\mathsf{mk}^2}{2(2\mathsf{j} + 1)^2} = -\frac{\mathsf{mk}^2}{2\mathsf{n}^2}, \tag{39}$$

where $n = 2j + 1$ is an integer.[3]

An important side note is, that this calculation was initially performed by Wolfgang Pauli in 1926 with minimal knowledge about today's quantum mechanical world. Indeed, in none of our calculations we used, for example, Schrödinger's equation. This example is perfect to show how powerful continuous symmetries are in solving physical and in particular quantum mechanical problems. [7]

4.4 Degeneracy

Now that we have calculated the energy eigenvalues of the hydrogen atom an interesting addition would be to look at their degeneracy and compare the result with the typical treatment of this problem. As we have seen in section 3.4, the irreducible representation V^{2j} of $\mathfrak{so}(3)$ (equivalent to the Hilbert space $\mathcal{H}_j$) has dimension $2j + 1$. In the above discussion we have seen that the eigenspace of the energy eigenvalues E_n is the $\mathfrak{so}(4)$ representation $\mathcal{H}_j \otimes \mathcal{H}_j$ with $n = 2j + 1$. Combining these facts we conclude that the degeneracy of the eigenvalue E_n is

$$\dim(\mathcal{H}_j \otimes \mathcal{H}_j) = (2j + 1)^2 = n^2 \tag{40}$$

The same result is achieved if we assume that the angular momentum quantum number l takes values between 0 and $n - 1$.

$$\sum_{l=0}^{n-1} \dim(\mathcal{H}_l) = \sum_{l=0}^{n-1} 2l + 1 = n(n-1) + n = n^2 \tag{41}$$

So not only can we predict the energy eigenvalues correctly, but even their degeneracy can be accurately determined simply by observing the symmetry.

5 Conclusion

Starting in the classical world, we used Noether's theorem and the implied connection to conserved quantities as a motivation to the power of continuous symmetries in physics. We learnt that Lie groups are used to represent continuous symmetries mathematically and found that their corresponding Lie algebras can be used – together with the exponential map – to simplify the calculation of (irreducible) representations. After deriving the Lie algebra $\mathfrak{so}(3)$ of the rotational symmetry in the hydrogen atom and investigating the isomorphism to the simple Lie algebra $\mathfrak{sl}(2, \mathbb{C})$ we derived the irreducible representations V^n. The exponential map then helped us to find the representations of the Lie group in the even $\mathfrak{sl}(2, \mathbb{C})$ representations $V^{n=2l}$ which we connected with the eigenspaces of the total angular momentum operator $\mathcal{H}_l$ known from quantum mechanics. Finally, based on the classical conservation law of the RL vector in Kepler-type problems, we reviewed how its quantum counterpart leads to exhibit a hidden $\mathfrak{so}(4)$ symmetry in the H-atom. In turn this allowed to deduce the exact spectrum, including both energy levels and degeneracies.

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