Lie Algebras and the Hidden Symmetries of the Hydrogen Atom

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Abstract

The purpose of this paper is to confer an understanding of Lie algebras and how they can be used to study objects in the quantum realm – namely, the symmetries of the Hydrogen atom. It is with this aim in mind that the author attempts to briefly introduce Lie algebras and their representations, the Casimir operator, the Schrodinger operator in the context of bound states of the Hydrogen atom, and, at last, the Hydrogen representations of the Lie algebra so(4). At this point, one can finally get a glimpse of the symmetric relations contained within the theory and can even uncover symmetries only available to that reader who is equipped with the tools detailed above.

Lie Algebras

We start by first defining real Lie algebras – the crux of this entire exposition.

Definition 1. *A* real Lie algebra *is a real vector space* $\mathfrak{g}$ *with a bracket operation:* $[\cdot,\cdot]\colon \mathfrak{g}\times\mathfrak{g}\to\mathfrak{g}$ *that satisfies for all* $A, B, C \in \mathfrak{g}$ *and* $r, s \in \mathbb{R}$*:*

1. *Asymmetry:* $[A, B] = -[B, A]$*;*
2. *Linearity in both components:* $[rA + sB, C] = r[A, C] + s[B, C]$ *and* $[A, rB + sC] = r[A, B] + s[A, C]$*;*
3. *The Jacobi Identity:* $[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$*. The bracket* $[\cdot,\cdot]$ *is called the* Lie bracket*, sometimes called the commutator*[1]*. If* $[A, B] = 0$*, then we say that* A *commutes with* B *or* A *and* B *commute.*

Big Idea: A real Lie algebra is just a vector space with an operation that satisfies some properties. An example would be the quaternions. Also, a subspace $W \subset V$, where V satisfies a Lie bracket. In this second case, we say that W inherits the Lie algebra structure from the larger algebra. We then call W a Lie subalgebra.

> **Example:** The set of $n \times n$ matrices with complex entries and with Lie bracket $[A, B] := AB - BA$ is a Lie algebra. This is often denoted $gl(n, \mathbb{C})$ and is called the general linear (Lie) algebra over the complex numbers. It is left to the reader to check that $gl(n, \mathbb{C})$ satisfies the criteria above.

An important subalgebra of $gl(2, \mathbb{C})$ is the special unitary algebra

$$su(2) := \{A \in gl(2, \mathbb{C})\colon A + A^* = 0, \mathit{Tr}(A) = 0\}.$$

One simply needs to show that $su(2)$ satisfies the Lie algebra criteria, and if it has already been shown for $gl(2, \mathbb{C})$, itself, it should be apparent that $su(2)$ will inherit the same structure.

A good intuition to have for $su(2)$ is as the set of derivatives at the identity of differentiable curves in the Lie group $SU(2)$. Or, analogously, $su(2)$ might be thought of as the vector space of possible velocities (at the identity

[1] Especially in subjects emphasizing Group Theory and Ring Theory

element I) of particles moving inside the Lie group $SU(2)$. Put yet another way, $su(2)$ is the tangent space to the manifold $SU(2)$ at the point I.

Theorem 1 (Spectral Theorem for su(2)). [2] *Consider an element A of $su(2)$. Then there is a real nonnegative number λ and a matrix $M \in SU(2)$ such that*

$$M^*AM = \begin{pmatrix} i\lambda & 0 \\ 0 & -i\lambda \end{pmatrix},$$

where M^* denotes the conjugate transpose of M.

Proposition 1. *Suppose $A \in su(2)$. Then for any $t \in \mathbb{R}$ we have $\exp(tA) \in SU(2)$. Furthermore, the derivative of the function $\exp(tA)$ with respect to t at $t = 0$ is A, itself.*

One might like to know at this point whether or not this relationship between Lie groups and certain Lie algebras extends past $SU(2)$. It turns out that it does! First, we say that $su(2)$ is the Lie algebra associated to $SU(2)$ and that it is unique. But there is also a unique Lie algebra associated to *any* Lie group. So knowing the Lie group with which one is working directly determines which Lie algebra one may consider! However, it's *not* true when going the other direction, i.e. a Lie algebra does not uniquely determine a Lie group[3].
Next, we consider the algebras $so(n)$, as we will later be using $so(3)$ and $so(4)$. Generally speaking,

$$so(n) := \{A \in gl(n, \mathbb{C})\colon A + A^T = 0 \text{ and all entries of } A \text{ are real}\}.$$

We will also be using the properties of Lie algebra homomorphism and isomorphism later on. Since these definitions are analogous to those of groups and representations, they will not be proved here.

Definition 2. *Suppose $\mathfrak{g}_1$ and $\mathfrak{g}_2$ are Lie algebras with bracket operations $[\cdot,\cdot]_1$ and $[\cdot,\cdot]_2$, respectively. Suppose T is a linear transformation from $\mathfrak{g}_1$*

[2]Note the subtle difference between *this* Spectral Theorem and that of $SU(2)$. It is expected that the reader has previously defined said theorem and will hopefully notice that – in this case – our element to be diagonalized, A, comes from the Lie algebra $su(2)$, while in the $SU(2)$ case, the analogous element U came from the Lie *group* $SU(2)$. This distinction between Lie algebras and Lie groups may seem inconsequential, but the reader who consistently makes an effort to recall the Lie algebra criteria above – whenever prudent – will benefit significantly.

[3]See exercise 8.5 in Singer's *Linearity, Symmetry, and Prediction in the Hydrogen Atom* [2005].

to $\mathfrak{g}_2$. Then T is a Lie algebra homomorphism if it respects the Lie bracket, i.e., if

$$[TA, TB]_2 = T([A, B]_1)$$

for every $A, B \in \mathfrak{g}_1$. If T is injective and surjective, then T is a Lie algebra isomorphism.

The reader is free to check that the three-dimensional subspace of the quaternions spanned by $\mathbf{i}, \mathbf{j}$, and $\mathbf{k}$, labeled here as $\mathfrak{g}_{\mathbf{Q}}$, is isomorphic to $su(2)$, which is ismorphic to $so(3)$. Also, $\mathfrak{g}_{\mathbf{Q}} \cong so(3)$, itself. For further use as we continue on, we wish to define $T_1 \colon \mathfrak{g}_{\mathbf{Q}} \to su(2)$ by

$$\begin{aligned}
T_1(\mathbf{i}) &= \frac{1}{2}\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \\
T_1(\mathbf{j}) &= \frac{1}{2}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \\
T_1(\mathbf{k}) &= \frac{1}{2}\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}.
\end{aligned}$$

We also wish to define $T_2 \colon \mathfrak{g}_{\mathbf{Q}} \to so(3)$ by

$$\begin{aligned}
T_2(\mathbf{i}) &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \\
T_2(\mathbf{j}) &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \\
T_2(\mathbf{k}) &= \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.
\end{aligned}$$

After checking that T_1 and T_2 are isomorphisms, we can conclude that $T_2 \circ T_1^{-1}$ is also an isomorphism. Thus, $su(2) \cong so(3)$.

Another crucial element of the so(4) analysis to which we are building will be the Cartesian sum of Lie algebras. First we will define them, and then the following proposition will illustrate why they are so essential to our study. Cartesian sums of Lie algebras are also quite similar to those with which the reader may be more familiar, so we will simply state the definition here.

Definition 3. *Suppose* $\mathfrak{g}_1$ *and* $\mathfrak{g}_2$ *are Lie algebras, with brackets* $[\cdot,\cdot]_1$ *and* $[\cdot,\cdot]_2$*, respectively. Then the Cartesian sum* $\mathfrak{g}_1 \oplus \mathfrak{g}_2$ *of vector spaces is a Lie algebra with bracket operation defined by*

$$[(A_1, A_2), (B_1, B_2)] := ([A_1, B_1]_1, [A_2, B_2]_2).$$

Proposition 2. *There is a Lie algebra isomorphism from* $su(2) \oplus su(2)$ *to* $so(4)$*.*[4]

The full proof of this proposition is omitted for brevity's sake. But the strategy is to define an isomorphism $S\colon \mathfrak{g}_{\mathbf{Q}} \oplus \mathfrak{g}_{\mathbf{Q}} \to so(4)$. Since we've already shown that $T_1\colon \mathfrak{g}_{\mathbf{Q}} \to su(2)$ is an isomorphism, we can use it to build our Cartesian product. After verifying that S is an isomorphism, we note that a composition of isomorphisms is itself an isomorphism. Thus, define

$$\begin{aligned} S \circ (T_1 \oplus T_1)^{-1}\colon su(2) \oplus su(2) &\to so(4) \\ (x, y) &\mapsto S(T_1^{-1}x, T_1^{-1}y). \end{aligned}$$

Representations of Lie Algebras

In this section, we will build our theory of Lie algebra representations, thereby further justifying our use of them as opposed to Lie groups, themselves. The definitions will be familiar to the reader who has studied group representations, and so we will again provide very little proof in an effort to achieve a modicum of concision.

Definition 4. *A Lie algebra homomorphism* ρ *from a Lie algebra* $\mathfrak{g}$ *to* $g\ell(V)$ *is called a* representation *of* $\mathfrak{g}$ *on* V*.*

Representations of Lie algebras follow the same notation as that of Lie groups, namely, we denote a representation by a triple $(\mathfrak{g}, V, \rho)$. Sometimes, this will be abbreviated to simply V or ρ.

[4] As an aside here, the reader may be wondering why it is that we even care about $so(4)$ to begin with. Essentially, studying the Hydrogen atom our natural space of states to which we are physically limited will only provide a full, clear picture of properties we can already "see". However, when we soon apply scrutiny in the context of $so(4)$, we will uncover some hidden symmetries whose theory we can study, but whose "visual" representations – to this day – remain a mystery. It is necessary to press on to fully convey the power of this toolkit, but hopefully this small justification will have motivated the reader to continue onward. We just have to add more tools, beforehand.

Definition 5. *Suppose* $(\mathfrak{g}, V, \rho)$ *and* $(\mathfrak{g}, \tilde{V}, \tilde{\rho})$ *are two representations of one Lie algebra* $\mathfrak{g}$*. Suppose* $T\colon V \to \tilde{V}$ *is a linear transformation such that for any* $v \in V$ *and any* $A \in \mathfrak{g}$*, we have*

$$T \circ \rho(A) = \tilde{\rho}(A) \circ T.$$

Then we say that T *is a* homomorphism of Lie algebra representations*. If – in addition –* T *is injective and surjective, then we say that* T *is an* isomorphism of Lie algebra representations *and that* ρ *is isomorphic to* $\tilde{\rho}$*.*

Considering that we're working with Lie algebras[5], we need to be careful when we perform calculations using partial derivatives. Simply put,

$$\partial_x(x\partial_y) = \partial_y + x\partial_x\partial_y \neq x\partial_x\partial_y = (x\partial_y\partial_x).$$

In other words, the partial differential doesn't commute in general. This will be important when we get to Runge-Lenz operators just before our final result.

We will be making use of a natural representation of the Lie algebra so(3) that uses partial differential operators on $L^2(\mathbb{R}^3)$. This will be the collection of our *angular momentum operators* in the form of linear transformations on $L^2(\mathbb{R}^3)$. These will be defined as:

$$\begin{aligned} \mathbf{L_i} &:= z\partial_y - y\partial_z \\ \mathbf{L_j} &:= x\partial_z - z\partial_x \\ \mathbf{L_k} &:= y\partial_x - x\partial_y \end{aligned}$$

There is a slight problem in the way that we've defined these operators – namely, that they are undefined for various elements of $L^2(\mathbb{R}^3)$. For the sake of precision[6], we let $W^\infty(\mathbb{R}^3)$ denote the subspace of infinitely differentiable functions in $L^2(\mathbb{R}^3)$ with every one of their derivatives also in $L^2(\mathbb{R}^3)$. Without getting too bogged down in details, we note that this is a dense subspace, so we can be assured it is well-defined and extrapolate from there to where we want to be. We define a function $\mathbf{L}\colon su(2) \to g\ell(W^\infty(\mathbb{R}^3))$ by:

$$\mathbf{L}(c_\mathbf{i}\mathbf{i} + c_\mathbf{j}\mathbf{j} + c_\mathbf{k}\mathbf{k}) := c_\mathbf{i}\mathbf{L_i} + c_\mathbf{j}\mathbf{L_j} + c_\mathbf{k}\mathbf{L_k}.$$

This $\mathbf{L}$ is the *total angular momentum.* One simply needs to check that it works well with the Lie brackets (which it does).

[5]...and since we can think of a Lie algebra as being the tangent space to the Lie group at the identity

[6]i.e. tedium

Definition 6. *Suppose* $\mathfrak{g}$ *is an arbitrary Lie algebra and* $(\mathfrak{g}, V, \rho)$ *is a Lie algebra representation. A subspace* W *of* V *is an* invariant subspace *for* ρ *if* $\rho(A)w \in W$ *for every* $A \in \mathfrak{g}$ *and every* $w \in W$. *If* W *is an invariant subspace for* ρ, *then the representation* $\rho_W \colon \mathfrak{g} \to g\ell(V)$ *defined by*

$$\rho_W(A) := \rho(A)|_W$$

is called a subrepresentation of ρ. *If* V *and* $\{0\}$ *are the only invariant subspaces of* V, *then we say that* $(\mathfrak{g}, V, \rho)$ *is an* irreducible representation.

Another result that carries over from the study of group representations is that, if T is a homomorphism of Lie algebra representations, then the kernel of T and the image of T are both invariant subspaces. Knowing this will allow us to talk about Schur's Lemma as applied to Lie algebra representations. [7]

Proposition 3. *Suppose* $(\mathfrak{g}, V_1, \rho_1)$ *and* $(\mathfrak{g}, V_2, \rho_2)$ *are irreducible representations of the Lie algebra* $\mathfrak{g}$. *Suppose that* $T \colon V_1 \to V_2$ *is a homomorphism of representations. Then there are only two possible cases:*

- *The function* T *is the zero function, or*
- *The representations* $(\mathfrak{g}, V_1, \rho_1)$ *and* $(\mathfrak{g}, V_2, \rho_2)$ *are isomorphic and* T *is an isomorphism.*

Proposition 4. [8] *Suppose* $\mathfrak{g}$ *is a Lie algebra and* $(\mathfrak{g}, V, \rho)$ *is a Lie algebra representation. Suppose* $T \colon V \to V$ *commutes with* ρ. *Then each eigenspace of* T *is an invariant space of the representation* ρ.

Proposition 5. [9] *Suppose* $(\mathfrak{g}, V_1, \rho_1)$ *and* $(\mathfrak{g}, V_2, \rho_2)$ *are two Lie algebra representations. Suppose* $T \colon V_1 \to V_2$ *is a homomorphism of representations. Then the image of* V_1 *under* T *is a subrepresentation of* V_2.

[7] It seems prudent to briefly mention here the concept of asymmetry between Lie algebras and Lie groups. It is true that every Lie group representation corresponds to a Lie algebra representation, however the converse is false. Note, there are no infinite-dimensional irreducible representations of the Lie group $SO(3)$ on complex scalar product spaces, but there are such representations of the corresponding Lie algebra $so(3)$. The reader may want to consider Lie groups as global objects, whereas Lie algebras are local objects. Simply put, just as there may be difficulty in pulling back a representation or in how there is ambiguity in an indefinite integral (with regard to constants), one can zoom into a local object, but zooming out isn't always possible. We will now introduce raising and lowering operators.

[8] This proposition will come in very handy near the end of our study.

[9] As will this one.

Raising Operators, Lowering Operators, and Irreducible Reps of su(2)

Here, we will construct a family of irreducible representations using an action of the Lie algebra on polynomials of two variables. These turn out to be the only finite-dimensional irreducible representations of $su(2)$, as all others will be isomorphic to one of them.

Since we can think of $su(2)$ as the real vector space spanned by $\{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$, with the Lie algebra bracket $[\mathbf{i}, \mathbf{j}] = \mathbf{k}$, $[\mathbf{j}, \mathbf{k}] = \mathbf{i}$, and $[\mathbf{k}, \mathbf{i}] = \mathbf{j}$, we can define a function $\mathbf{U}$ that will preserve the degree of homogeneous polynomials. For any $c_\mathbf{i}, c_\mathbf{j}, c_\mathbf{k} \in \mathbb{R}$, define $\mathbf{U}\colon su(2) \to g\ell(\mathcal{P})$ by

$$\mathbf{U}(c_\mathbf{i}\mathbf{i} + c_\mathbf{j}\mathbf{j} + c_\mathbf{k}\mathbf{k}) := c_\mathbf{i}\mathbf{U}_\mathbf{i} + c_\mathbf{j}\mathbf{U}_\mathbf{j} + c_\mathbf{k}\mathbf{U}_\mathbf{k},$$

with

$$\begin{aligned} \mathbf{U}_\mathbf{i} &:= i(x\partial_x - y\partial_y)/2 \\ \mathbf{U}_\mathbf{j} &:= (x\partial_y - y\partial_x)/2 \\ \mathbf{U}_\mathbf{k} &:= i(x\partial_y + y\partial_x)/2 \end{aligned}$$

Because $\mathbf{U}$ preserves the degree of homogeneous polynomials, each space $\mathcal{P}^n$ of degree n is a subrepresentation of $(su(2), \mathcal{P}, \mathbf{U})$. On top of that, the operators $\mathbf{U}_\mathbf{i}, \mathbf{U}_\mathbf{j}, \mathbf{U}_\mathbf{k}$ form an irreducible representation of $su(2)$ on $\mathcal{P}^n$, where n is nonnegative. To convince the reader of this, we must employ the eigenvectors of $\mathbf{U}_\mathbf{i} = \frac{i}{2}(x\partial_x - y\partial_y)$ on $\mathcal{P}^n$, which are

$$-\frac{in}{2}, i - \frac{in}{2}, \ldots, \frac{in}{2} - i, \frac{in}{2}.$$

We will also make use of the raising and lowering operators defined below.

Definition 7. *The* raising operator for the representation $\mathbf{U}$ *is defined as*

$$\mathbf{X} := \mathbf{U}_\mathbf{j} - i\mathbf{U}_\mathbf{k} = x\partial_y.$$

The lowering operator for the representation $\mathbf{U}$ *is*

$$\mathbf{Y} := \mathbf{U}_\mathbf{j} + i\mathbf{U}_\mathbf{k} = -y\partial_x$$

As you will see, these operators act on the space of polynomials of degree n in such a way that $\mathbf{X}$ raises the degree of the x variable and simultaneously lowers the degree of the y variable, while $\mathbf{Y}$ raises the exponent on y and lowers it on x. For example,

$$\mathbf{X}(x^k y^{n-k}) = (n-k)x^{k+1}y^{n-k-1}$$

and

$$\mathbf{Y}(x^k y^{n-k}) = -kx^{k-1}y^{n-k+1}$$

$\mathbf{X}$ shifts the focus "up" from eigenvalue $i(2k-n)/2$ to $i(2k-n)/2+i$, while $\mathbf{Y}$ shifts the focus "down." $\mathbf{X}$ and $\mathbf{Y}$ also preserve invariant subspaces, a fact the reader may wish to check on their own.

These operators were a specific case designed to familiarize the student with the concept of raising and lowering. More generally, we have the following definition.

Definition 8. *Suppose $(su(2), V, \rho)$ is a Lie algebra representation. Define the* raising operator for ρ *by*

$$\mathbf{X}_\rho := \rho(\mathbf{j}) - i\rho(\mathbf{k})$$

and the lowering operator for ρ *by*

$$\mathbf{Y}_\rho := \rho(\mathbf{j}) + i\rho(\mathbf{k}).$$

Proposition 6. *Suppose $(su(2), V, \rho)$ is a Lie algebra representation. Then $[\mathbf{X}_\rho, \mathbf{Y}_\rho] = 2i\rho(\mathbf{i})$. Furthermore, if $v \in V$ is an eigenvector for $\rho(\mathbf{i})$ with eigenvalue λ, then*

$$\rho(\mathbf{i})(\mathbf{X}_\rho v) = (\lambda + i)\mathbf{X}_\rho v$$
$$\rho(\mathbf{i})(\mathbf{X}_\rho v) = (\lambda - i)\mathbf{X}_\rho v$$

It is not necessarily true that $\lambda + i$ is an eigenvalue of $\rho(\mathbf{i})$, nor is it necessarily true that $\lambda - i$ is, either. Respectively, $\mathbf{X}_\rho v$ might be 0, or $\mathbf{Y}_\rho v$ might be 0. This seems frustrating because we aren't able to check all possible values. However, using with the following definition and the next two propositions, we can speed around this problem. The reader will consider the Lie algebra bracket $[\mathbf{X}_\rho, \mathbf{Y}_\rho]$ and will conclude that either $\mathbf{X}_\rho v = 0$, or $\mathbf{X}_\rho v$ is an eigenvector of $\rho(\mathbf{i})$ with eigenvalue $\lambda + 1$. Similarly, we have either $\mathbf{Y}_\rho v = 0$ or $\mathbf{Y}_\rho v$ is an eigenvector with eigenvalue $\lambda - i$. We will then see – because of the concept of highest weight vectors (defined below) – we are able to generate irreducible subprepresentations. This is analogous to the work done above for the case of $\mathcal{P}^n$.

Definition 9. *Suppose* $(su(2), V, \rho)$ *is a finite-dimensional Lie algebra representation. Suppose* v_0 *is an eigenvector of* $\rho(\mathbf{i})$ *with the property that* $\mathbf{X}_\rho v_0 = 0$*. Then* v_0 *is a* highest weight vector for the representation ρ.

Proposition 7. *Suppose* $(su(2), V, \rho)$ *is a finite-dimensional Lie algebra representation. Then there exists at least one highest weight vector for* ρ *in* V*. Suppose* v_0 *is a highest weight vector for* ρ*. Then there is a unique non-negative integer* n *such that* $\mathbf{Y}_\rho^n v_0 \neq 0$ *and* $\mathbf{Y}_\rho^{n+1} = 0$*. For any* $k = 0, \ldots, n$*, we have*

$$\rho(\mathbf{i})\mathbf{Y}_\rho^k v_0 = \frac{i}{2}(n - 2k)\mathbf{Y}_\rho^k v_0.$$

Furthermore,

$$\{\mathbf{Y}_\rho^k v_0 \colon k = o, \ldots, n\}$$

is a basis for an irreducible subrepresentation W *of* V*.*

Proposition 8. *Suppose* $(su(2), V, \rho)$ *is a finite-dimensional irreducible Lie algebra representation. Set*

$$n := \dim V - 1.$$

Then $(su(2), V, \rho)$ *is isomorphic to the representation* $(su(2), \mathcal{P}^n, \mathbf{U})$*.*

It is because of the two propositions above that we are able to consider the eigenvectors of $\mathbf{U_i}$ in the first place. We like that because, unlike $\rho(\mathbf{i})$, we don't get any false eigenvalues. In a way, the set of eigenvalues for $\mathbf{U_i}$ is dense, while that of $\rho(\mathbf{i})$ is not.

In order to classify the representations of $su(2)$, we need to decide on a way in which to *identify* them. The Casimir operator will prove itself useful to this end.

The Casimir Operator and Irreducible Reps of so(4)

Definition 10. *Suppose* $(su(2), V, \rho)$ *is a Lie algebra representation. The* Casimir operator *for* ρ *is the linear transformation* $\mathbf{C} \colon V \to V$ *defined by*

$$\mathbf{C} := \rho(\mathbf{i})^2 + \rho(\mathbf{j})^2 + \rho(\mathbf{k})^2.$$

Notice that the Casimir operator doesn't correspond to elements in the Lie algebra with which we're working, but rather the general linear group of the vector space in our representation. Thus, in order to define a Casimir operator, we need a representation. Crucially, the Casimir operator commutes with everything in the image of said representation.

Proposition 9. [10] *Suppose $(su(2), V, \rho)$ is a representation and $\mathbf{C}$ is its Casimir operator. Then $\mathbf{C}$ commutes with ρ.*

Proposition 10. *Suppose $(su(2), V, \rho)$ is a finite-dimensional irreducible Lie algebra representation. Then the Casimir operator is a scalar multiple of the identity on V.*

This proof makes use of the fact that each finite-dimensional irreducible representation of $su(2)$ is isomorphic to $\mathcal{P}^n$ for some n. After some computation, it is discovered that $\mathbf{C} = -\frac{1}{4}(n^2 + 2n)I$, which will be important later on.

Proposition 11. *Suppose $(su(2), V, \rho)$ is a finite-dimensional Lie algebra representation. Suppose $\mathbf{C} = -\ell(\ell + 1)I$ on V for some nonnegative half-integer*[11] *ℓ. Then the eigenvalues of $\rho(\mathbf{i})\colon V \to V$ are*

$$\{-i\ell, -i\ell + 1, \ldots, i\ell - i, i\ell\}$$

Using the natural representation on a tensor product, we seek to classify irreducible representations of $su(2) \oplus su(2)$ using the concept of Casimir operators.

Definition 11. [12] *Suppose $(\mathfrak{g}_1, V_1, \rho_1)$ and $(\mathfrak{g}_2, V_2, \rho_2)$ are two representations of a Lie algebra $\mathfrak{g}$. Then the* tensor product *of the two representations is*

$$(\mathfrak{g}_1 \oplus \mathfrak{g}_2, V_1 \otimes V_2, \rho_1 \otimes I + I \otimes \rho_2),$$

where

$$(\rho_1 \otimes I + I \otimes \rho_2)(A, B) := \rho_1(A) \otimes I + I \otimes \rho_2(B)$$

for any $A \in \mathfrak{g}_1$ and $B \in \mathfrak{g}_2$.

The next proposition uses the fact that $so(4) \cong su(2) \oplus su(2)$ in an effort to classify finite-dimensional irreducible representations of the Lie algebra $so(4)$. Because of this isomorphism, is is sufficient to classify such representations of $su(2) \oplus su(2)$, which is easier.

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[10] The proof of this proposition simply involves algebra on the brackets $[\mathbf{C}, \rho(\mathbf{i})], [\mathbf{C}, \rho(\mathbf{j})]$, and $[\mathbf{C}, \rho(\mathbf{k})]$ and is thus omitted here. In fact, from this point on, if a proof is omitted, it may be assumed to be similar to one similar in the context of Lie groups.

[11] Physicists may be more familiar with this term. For the rest of us, the clue is in the title, but it helps to see it defined: a half-integer $\ell := \frac{n}{2}$, where n is an integer.

[12] If this definition looks gross, try thinking about the Lie algebra as the space of derivatives of a Lie group at the identity. Then, the expression $\rho_1(\mathbf{q}) \otimes I + I \otimes \rho_2(\mathbf{p})$ looks like nothing more than the product rule learned way back in an early Calculus course.

Proposition 12. *Suppose* $(su(2) \oplus su(2), V, \rho)$ *is a finite-dimensional irreducible representation. Then there are irreducible representations*

$$(su(2), W_1, \rho_1) \text{ and } (su(2), W_2, \rho_2)$$

such that the representation $(su(2) \oplus su(2), V, \rho)$ *is isomorphic to the Lie algebra representation*

$$(su(2) \oplus su(2), W_1 \otimes W_2, \rho_1 \otimes I + I \otimes \rho_2)$$

This is all pretty powerful stuff. We've taken a fairly simple Lie algebra $su(2)$ and used it, along with the Casimir operator, the classify irreducible representations of $so(4)$. We now have most of the necessary mathematics out of the way and will move into more of a physics-oriented[13] landscape. As such, we begin the next section introducing some terminology for the non-physicist.

Bound States of the Hydrogen Atom

The *bound states* of the hydrogen atom are the states such that the electron stays with the nucleus, whereas in the *unbound states*, the electron has enough energy to simply speed past the nucleus without getting trapped in the shell. We are only concerned with the bound states, as the unbound electron doesn't remain within the shell long enough to form an atom worth studying for our current purposes.

Definition 12. *The Schrodinger*[14] *operator is defined as*

$$\mathbf{H} := -\frac{\hbar^2}{2\mathbf{m}}(\partial_x^2 + \partial_y^2 + \partial_z^2) - \frac{\mathbf{e}^2}{\sqrt{x^2 + y^2 + z^2}},$$

where $\mathbf{e}$ *is the charge of the electron and* $\mathbf{m}$ *is its mass.*

Recall the symbol $\hbar$ is Planck's constant divided by 2π. As an aside, the expression

$$\frac{\mathbf{e}^2}{\sqrt{x^2 + y^2 + z^2}}$$

[13] We can do this because the result is the same regardless of orientation. ☺

[14] Readers may note the absence of the umlaut over the o. Some alphabet packages are not natively included and must be defined manually on some computers. I'm not defining a macro for an umlaut...

is called the Coulomb potential, which is essentially only usable in the case of our Hydrogen atom. Were we to study an atom with more electrons, we would need more quantum theory and less classical physics – in which case we would be unable to make much sense of the Coulomb potential and would hopefully have some other tools at our disposal.[15] Luckily, we *are* studying the Hydrogen atom and will soldier onward with our Schrodinger operator. With it, we can make predictions about energy levels in a hydrogen atom. Suppose $\phi \in L^2(\mathbb{R}^3)$ satisfies the following equation

$$\mathbf{H}\phi = E\phi$$

for some real number E. This is the Schrodinger eigenvalue equation and when ϕ satisfies it, we can write

$$-\frac{\hbar^2}{\mathbf{2m}}(\nabla^2\phi)(x,y,z) - \frac{\mathbf{e}}{\sqrt{x^2+y^2+z^2}}\phi(x,y,z) = E\phi(x,y,z).$$

Now, if we consider an electron in such a state ϕ, then a measurement on said electron will give us the energy, E. Thus, the eigenvalues of the Schrodinger operator are known as energy eigenvalues or energy levels, and the eigenfunctions corresponding to them are called energy eigenstates. Our interest here lies in the vector space spanned by the eigenstates that have negative energy values. [16]

Proposition 13. [17] *Each negative eigenvalue E of the Schrodinger operator has a finite number of linearly independent eigenfunctions.*

Note that for any $g \in SO(3)$ and any f in the domain of $\mathbf{H}$, we must have $\mathbf{H} \circ \rho(g) = \rho(g) \circ \mathbf{H}$. This commutativity is required due to the spherical symmetry of the physical space. $\mathbf{H}$ does indeed commute with such angular

[15]To begin such a study, the author recommends Rouvray's *The Mathematics of the Periodic Table*.

[16]There's more to it than that, but a short explanation is thus: essentially, the Coulomb potential tends to 0 as $x^2 + y^2 + z^2$ gets larger, thus 0 simply makes sense as an upper bound. Take a particle with positive energy and it will break out of the scope of our study, whereas a particle with negative energy will correspond to an electron that remains with it's atom's nucleus – just what we're interested in.

[17]The proof of this proposition is actually the first such proof that can be considered beyond the scope of the material presented, so – rather than tell the reader to recall an idea from the theory of Lie groups, as in the case of prior excluded proofs – it is wise for the reader to construct an intuitive sense of what this proposition says. Maybe one could recall just the concept of separation of variables and its relation to radial and angular components of wave functions.

momentum operators, as the reader may wish to verify. This shows us that, when restricted to a single eigenspace of the Schrodinger operator, the angular momentum operators form a representation of $su(2)$. There will be one of these representations for each eigenvalue of $\mathbf{H}$, and we can put them together to form a representation of $su(2)$ on the vector space of bound states of the hydrogen atom. And then, in our next section, we will see a natural representation of $so(4)$, which the reader will again recall is isomorphic to $su(2) \oplus su(2)$.

The Hydrogen Representations of $so(4)$

Using the representation theory of the Lie algebra $so(4)$, we can make a prediction about the dimensions of the shells of the hydrogen atom, as well as the energy levels of these shells. This is something we are able to do due to the representation theory, itself, and the fact that there exists a representation of $so(4)$ on the space of bound states of the Schrodinger operator.

First, we define a set of operators that, like the angular momentum operators, commute with the Schrodinger operator. These are only defined on the bound states of $\mathbf{H}$ and the way in which they are useful depends on the Coulomb potential described above.

Definition 13. *The* Runge-Lenz operators *are defined as follows:*

$$\mathbf{R_i} := \frac{i\hbar}{\sqrt{-8\mathbf{m}E}} \left(\mathbf{L_k}\partial_y + \partial_y \mathbf{L_k} - \mathbf{L_j}\partial_z - \partial_z \mathbf{L_j} + \frac{2\mathbf{me}^2 x}{\hbar^2 \sqrt{x^2+y^2+z^2}} \right)$$
$$\mathbf{R_j} := \frac{i\hbar}{\sqrt{-8\mathbf{m}E}} \left(\mathbf{L_i}\partial_z + \partial_z \mathbf{L_i} - \mathbf{L_k}\partial_x - \partial_x \mathbf{L_k} + \frac{2\mathbf{me}^2 x}{\hbar^2 \sqrt{x^2+y^2+z^2}} \right)$$
$$\mathbf{R_k} := \frac{i\hbar}{\sqrt{-8\mathbf{m}E}} \left(\mathbf{L_j}\partial_x + \partial_x \mathbf{L_j} - \mathbf{L_i}\partial_y - \partial_y \mathbf{L_i} + \frac{2\mathbf{me}^2 x}{\hbar^2 \sqrt{x^2+y^2+z^2}} \right).$$

On the vector space of bound states, we can form a representation of $so(4)$ by combining the Runge-Lenz operators and the angular momentum operators.
Our strategy will be as follows: consider a single eigenspace of $\mathbf{H}$. Then, fix an eigenvalue E (which must be negative). Let V_E denote the eigenspace corresponding to E. We have already determined that there is a representation of $su(2)$ on V_E, and we will extend this to a representation of $su(2) \oplus su(2)$.

Upon calculating the Lie brackets for these operators, we see that

$$[\mathbf{R_i}, \mathbf{R_j}] = \mathbf{L_k}$$
$$[\mathbf{R_j}, \mathbf{R_k}] = \mathbf{L_i}$$
$$[\mathbf{R_k}, \mathbf{R_i}] = \mathbf{L_j}.$$

The reader should also note that

$$\mathbf{L} \cdot \mathbf{R} = \mathbf{R} \cdot \mathbf{L} = 0.$$

There is a lot of algebraic manipulation that we will skip over as we go on to introduce the representation of $so(4)$. Define

$$\mathbf{A_i} := (\mathbf{L_i} + \mathbf{R_i})/2 \qquad \mathbf{B_j} := (\mathbf{L_j} - \mathbf{R_j})/2$$
$$\mathbf{A_j} := (\mathbf{L_j} + \mathbf{R_j})/2 \qquad \mathbf{B_i} := (\mathbf{L_i} - \mathbf{R_i})/2$$
$$\mathbf{A_k} := (\mathbf{L_k} + \mathbf{R_k})/2 \qquad \mathbf{B_k} := (\mathbf{L_k} - \mathbf{R_k})/2$$

It follows from here that

$$[\mathbf{A_i}, \mathbf{A_j}] = \mathbf{A_k},$$
$$[\mathbf{A_j}, \mathbf{A_k}] = \mathbf{A_i},$$
$$[\mathbf{A_k}, \mathbf{A_i}] = \mathbf{A_j},$$

and similarly,

$$[\mathbf{B_i}, \mathbf{B_j}] = \mathbf{B_k}.$$
$$[\mathbf{B_j}, \mathbf{B_k}] = \mathbf{B_i}.$$
$$[\mathbf{B_k}, \mathbf{B_i}] = \mathbf{B_j}.$$

Our **A** set forms a representation of $su(2)$, as does our set of **B**'s. So from what we've learned in previous sections, we can construct a representation of $su(2) \oplus su(2)$[18], which is isomorphic to $so(4)$. Hence, we have a representation of $so(4)$.

[18] The commutative property can be illustrated with more bracket algebra.

Finally, we can start using all that we've constructed above. We are going to calculate the value of the Casimir operator for the representations of $su(2)$. Since $\mathbf{L} \cdot \mathbf{R} = \mathbf{R} \cdot \mathbf{L} = 0$ we have

$$\mathbf{A}^2 = \mathbf{B}^2 = \frac{1}{4}(\mathbf{L}^2 + \mathbf{R}^2) = \frac{1}{4}\left(1 + \frac{\mathbf{me}^2}{2E\hbar^2}\right).$$

It should be recalled that the Casimir operator determines an irreducible representation of $su(2)$. We learned above that the value of the Casimir is $-\frac{1}{4}(n^2 + 2n)$, for nonnegative integer n. Thus,

$$-(n^2 + 2n) = 1 + \frac{\mathbf{me}^4}{2E\hbar^2},$$

which means that the eigenvalues of the Schrodinger operator are of the form

$$E = \frac{\mathbf{me}^4}{2\hbar^2(n+1)^2}.$$

Note that the eigenspace corresponding to this eigenvalue is made up of irreducible representations of $so(4)$ isomorphic to $\mathcal{P}^n \otimes \mathcal{P}^n$. So, because the dimension is finite, the dimension of the eigenspace is an integer multiple of the dimension of $\mathcal{P}^n \otimes \mathcal{P}^n$, which is $(n+1)^2$. This gives that the lowest eigenvalue is $-\mathbf{me}^4/2$ and the eigenspace associated with it must have dimension divisible by 1. The next lowest possible eigenvalue is $-\mathbf{me}^4/8$ and it must have eigenspace with dimension divisible by 4. The pattern continues in this fashion with $-\mathbf{me}^4/18$ with eigenspace divisible by 9. Experimental evidence concurs with this result and so we have illustrated how representation theory can predict that the dimensions of the irreducible representations of $so(4)$ divide the multiplicities of the respective energy levels in the hydrogen atom. The prediction – albeit, off by a factor of two due to the spin of the electron[19] – is backed by the power of isomorphisms of representations. All calculations performed to get from beginning to end are just clever algebraic manipulations with a set of defined operators, and without loss of generality.

Conclusion

The wonder that we've discovered may seem minuscule at first glance. But upon further consideration, we've really come up with a way to make the

[19]For more on spin, see chapter 10 of Singer [2005]

entire concept of higher-dimensional space more tangible. We've taken something that exists in our own 3-D world and learned that, when we place it in a larger box – one that possibly allows it to stretch and move about more freely – it clearly makes use of the extra dimension. As for what it gets up to, that is still a mystery.

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