Understanding Quantum Mechanical Systems with Spherical Symmetry via Representations of Lie Groups

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Introduction

> *"I think I can safely say that nobody understands quantum mechanics."*
> —Richard Feynman (1965)

It is a sorry state of affairs in which one of a field's most brilliant thinkers claims that field is impossible to understand. Granted, Richard Feynman was not saying that the mathematics describing quantum physics was unknown—he certainly was as familiar with it as anyone—but that the physics itself is deeply counterintuitive and demands a shift in perception in order to internalize it. Still, this sentiment that quantum mechanics is 'too difficult' to understand persists because undergraduate physics students usually do not possess the necessary mathematical background for a complete understanding of quantum phenomena. Such a difficulty is unavoidable, as professors cannot be expected to go on lengthy digressions into Lie theory, but it is lamentable nonetheless.

My goal in this paper is to ease the confusion, at least partially, by providing a rigorous mathematical explanation of angular momentum and spin accessible to an undergraduate physics or mathematics major. We will introduce representation theory as it relates to Lie groups and Lie algebras. Then we will focus on the two Lie groups SU(2) (the special unitary group of order two) and SO(3) (the special orthogonal group of order three), which are of great importance in the theory of angular momentum. Finally we will relate these groups to angular momentum by reproducing the calculations that appear in introductory quantum mechanics textbooks in a more thorough manner.

We will not assume any familiarity with Lie theory, although a basic understanding of concepts in quantum mechanics such as probability amplitudes, spin, etc. is important. Familiarity with linear algebra and basic group theory is assumed. Section 1 provides a short explanation of the relevant physics and explains our goal: to describe the solutions of a quantum mechanical system with spherical symmetry. Section 2 provides the necessary background in Lie theory, and Section 3 applies these results to the groups SU(2) and SO(3). Section 4 discusses the irreducible representations of SU(2), SO(3), and their Lie algebras, while Section 5 applies these results to spin and angular momentum.

1 Angular Momentum and the Schrodinger Equation

1.1 The Schrödinger Equation

The goal of our analysis is to find solutions $\psi : \mathbb{R}^3 \to \mathbb{C}$ to the **time-independent Schrödinger equation (TISE)**:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x}) + V(\mathbf{x})\psi(\mathbf{x}) = E\psi(\mathbf{x}) \tag{1}$$

where $\hbar$ and m are constants, $V : \mathbb{R}^3 \to \mathbb{R}$ is the potential energy function, and E is the system's energy. Any student of quantum mechanics knows the solution $\psi(\mathbf{x})$ as the wavefunction of the system and that the square modulus of $\psi(\mathbf{x})$ gives a probability density function for the location of the particle $\psi(\mathbf{x})$ describes. Thus solutions to equation (1) are elements of $L^2(\mathbb{R}^3, \mathbb{C})$, the space of square-integrable complex-valued functions on $\mathbb{R}^3$. However, we will not dwell on this point, but instead emphasize the fact that the codomain is $\mathbb{C}$.

The left-hand side of equation (1) is often considered as an operator $\hat{H}$ (the Hamiltonian) acting on $\psi(\mathbf{x})$, in which case the TISE becomes an eigenvalue equation for $\hat{H}$:

$$\hat{H}\psi(\mathbf{x}) = E\psi(\mathbf{x}). \tag{2}$$

The Hamiltonian is the 'energy operator,' and from this point of view our goal is to find the eigenfunctions and eigenvalues of $\hat{H}$. Ultimately, these eigenfunctions are seen to be the states of the system with well-defined energies. Linear combinations of the eigenfunctions are solutions to the **Time-dependent Schrödinger equation (TDSE)**, which describes the evolution of the system over time. However, a thorough discussion of the TDSE is outside of the scope of this text, so we restrict our attention to finding the eigenfunctions of the TISE.

We will focus on a particular case of the Schrödinger equation—namely when $V(\mathbf{x})$, and hence $\hat{H}$, has rotational symmetry (the Laplacian, ∇^2 is always rotationally invariant). By rotational symmetry we mean that rotating one solution to the system produces another solution. Many important physical systems, most notably the hydrogen atom, have rotational symmetry, so an analysis of the rotationally invariant Schrödinger equation covers much ground in quantum mechanics. Moreover, its analysis is made simpler by the property of angular momentum, which we now introduce.

1.2 Angular Momentum

In classical mechanics, the angular momentum of a particle is defined as the cross product of the particle's displacement $\mathbf{r}$ (with respect to some reference frame) and its momentum $\mathbf{p}$:

$$\mathbf{L} = \mathbf{r} \times \mathbf{p},$$

which is to say,

$$L_1 = x_2p_3 - x_3p_2, \quad L_2 = x_3p_1 - x_1p_3, \quad \text{and} \quad L_3 = x_1p_2 - x_2p_1.$$

We may extend this definition to quantum mechanics using the quantum mechanical position and momentum operators:

$$\hat{\mathbf{x}} = \mathbf{x}, \quad \text{and} \quad \hat{\mathbf{p}} = -i\hbar\nabla,$$

which gives us

$$L_1 = -i\hbar\left(x_2\frac{\partial}{\partial x_3} - x_3\frac{\partial}{\partial x_2}\right); \quad L_2 = -i\hbar\left(x_3\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_3}\right);$$
$$L_3 = -i\hbar\left(x_1\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_1}\right). \tag{3}$$

Note that because different components of $\hat{x}$ and $\hat{p}$ commute, these operators are well defined.

The angular momentum operators may be thought of as infinitesimal rotations (or generators of rotations) in the following manner. If we change to spherical coordinates with $\theta = 0$ pointing along the x_3-axis, then we may write

$$L_3 = -i\hbar \frac{d}{d\phi}\psi(R_\phi \mathbf{x})\bigg|_{\phi=0},$$

where R_ϕ is a counterclockwise rotation by angle ϕ in the (x_1, x_2) plane. L_1 and L_2 may similarly be expressed via rotations about their respective coordinate axes. Later, after we discuss Lie group and Lie algebra representations, we will find that the angular momentum operators define the representation of the Lie algebra associated to the natural representation of the Lie group SO(3) on the space of three-dimensional wavefunctions.

To elaborate on this connection between angular momentum and rotations, we introduce the bracket (or commutator) defined as $[X, Y] = XY - YX$ for quantum mechanical operators X and Y. We note two important facts about the commutator.

Proposition 1.1. *The three angular momentum operators obey the following commutation relations:*

$$[L_1, L_2] = i\hbar L_3; \quad [L_2, L_3] = i\hbar L_1; \quad [L_3, L_1] = i\hbar L_2. \tag{4}$$

These are precisely the commutation relations of the Lie algebra so(3) *associated to the Lie group* SO(3) *(see Section 3)*

Proof. We use the canonical commutation relation $[x_i, p_i] = i\hbar$ (for $i = 1, 2, 3$). For L_1 and L_2, we have

$$\begin{aligned}[L_1, L_2] &= [x_2p_3 - x_3p_2, x_3p_1 - x_1p_3] \\ &= x_2[p_3, x_3]p_1 + [x_3, p_3]p_2x_1 \\ &= i\hbar(x_1p_2 - x_2p_1) = i\hbar L_3.\end{aligned}$$

The other two commutation relations can be obtained in a similar manner. Note it is also possible to derive this result by multiplying out the differential expressions for L_1 and L_2 and then cancelling like terms (which works because second order partial derivatives do not depend on the order of differentiation). □

A second point about the commutator is of fundamental importance. If the commutator of two operators is zero (i.e., if they commute), then the operators have a complete set of mutual eigenfunctions, meaning that all solutions to the system are linear combinations of the mutual eigenfunctions. This we will not prove (though it is not difficult to show), but the following corollary is important to our discussion.

Proposition 1.2. *In a rotationally invariant quantum mechanical system, the invariant subspaces of the Hamiltonian $\hat{H}$ are also invariant subspaces of the angular momentum operators L_1, L_2, and L_3.*

Proof. In general we have that any rotation of a solution $\psi(\mathbf{x})$ will give another solution to the time-independent Schrödinger equation. In particular this is true for any rotation around the x_3-axis. Consider an infinitesimal rotation by angle $d\theta$:

$$\begin{aligned} x_1' &= x_1 + d\theta x_2, \\ x_2' &= x_2 - d\theta x_1, \\ x_3' &= x_3. \end{aligned}$$

Plugging these new values into $\psi(\mathbf{x})$ gives a new solution to the TISE:

$$\hat{H}\psi(x_1 + d\theta x_2, x_2 - d\theta x_1, x_3) = E\psi(x_1 + d\theta x_2, x_2 - d\theta x_1, x_3). \tag{5}$$

Expanding equation (5) as a Taylor series, we find

$$\hat{H}\psi(x_1, x_2, x_3) + \hat{H}d\theta\left(\frac{\partial\psi}{\partial x_1}x_2 - \frac{\partial\psi}{\partial x_2}x_1\right) = E\psi(x_1, x_2, x_3) + Ed\theta\left(\frac{\partial\psi}{\partial x_1}x_2 - \frac{\partial\psi}{\partial x_2}x_1\right)$$

which gives, when we subtract off equation (2),

$$\hat{H}\left(\frac{\partial}{\partial x_1}x_2 - \frac{\partial}{\partial x_2}x_1\right)\psi = \left(\frac{\partial}{\partial x_1}x_2 - \frac{\partial}{\partial x_2}x_1\right)\hat{H}\psi.$$

Multiplying both sides of the equation by $-i\hbar$ we see that $[\hat{H}, L_3] = 0$ as desired. The same argument using rotations around the x_1 and x_2-axes shows that L_1 and L_2 commute with $\hat{H}$ as well. □

Because $\hat{H}$ and L_3 commute, they share eigenfunctions, and thus we can solve equation (2) by finding the eigenfunctions and eigenvalues of L_3. In other words, we are able to find solutions to the rotationally invariant Schrödinger equation simply by performing an analysis of angular momentum. The next two sections are devoted to the theory of Lie groups, which will provide the necessary mathematical background to discuss angular momentum in detail.

2 Lie Theory

Lie groups are in some sense the natural mathematical structure to use when studying systems with continuous symmetry (e.g., rotational symmetry) because the operation under which the system is invariant can then be viewed as an action of a Lie group on the space. For our discussion, the relevant Lie groups are the special orthogonal group of order three, SO(3), and the special unitary group of order two, SU(2). SO(3) can be viewed as the group of rotations of three-dimensional real Euclidean space, while SU(2) can be viewed as the group of rotations of two-dimensional complex Euclidean space. The two groups are related to each other by a 2-1 and onto homomorphism from SU(2) to SO(3) (in topological jargon, SU(2) is the universal cover of SO(3)).

We begin by introducing the necessary mathematical background to discuss these two groups. In particular we would like to discuss how these two groups relate to each other, their properties as Lie groups (smooth groups with smooth group operations), and representations of the groups and their Lie algebras. In this discussion we omit extraneous details and proofs, instead focusing solely on the theory relevant to angular momentum. By the end of this section we will have introduced matrix Lie groups, Lie algebras, the matrix exponential, representations, and various important properties of these objects. For those interested in seeing the theory of Lie groups and Lie algebras laid out in detail, many of the proofs of our results can be found in [1]. In the next section we will make this discussion concrete by applying our results to SU(2) and SO(3).

2.1 Lie Groups

In general, a Lie group is a smooth manifold with smooth group operations, but here we focus on a subclass of Lie groups which we call matrix Lie groups—essentially Lie groups that can be represented as a set of matrices. Formally these groups are closed subgroups of the group of invertible matrices over $\mathbb{C}$.

Definition 2.1. The **general linear group** over the complex numbers, denoted $\mathrm{GL}(n;\mathbb{C})$, is the group of all $n \times n$ invertible matrices with complex entries.

Definition 2.2. For any $X \in M_n(\mathbb{C})$, we define the **Hilbert-Schmidt** norm of X to be the quantity

$$||X|| = \left(\sum_{j,k=1}^{n} |X_{jk}|^2 \right)^{1/2},$$

which may be computed in a basis independent way as $||X|| = (\mathrm{trace}(X^* X))^{1/2}$.

Definition 2.3. A **matrix Lie group** is a closed subgroup G of $\mathrm{GL}(n;\mathbb{C})$, i.e., if A_m is any sequence of matrices in G and A_m converges to some matrix A (in the Hilbert-Schmidt norm), then either A is in G or A is not invertible.

In any discussion of groups there must be some notion of a group homomorphism. For Lie groups, homomorphisms are defined in the usual way with continuity as an added condition.

Definition 2.4. Let G and H be matrix Lie groups. A map $\Phi : G \to H$ is called a **Lie group homomorphism** if (1) $\Phi(X_1X_2) = \Phi(X_1)\Phi(X_2)$ for all $X_1, X_2 \in G$ (i.e., Φ is a group homomorphism) and (2) Φ is continuous. If, in addition, Φ is one-to-one and onto and the inverse map Φ^{-1} is continuous, then Φ is called a **Lie group isomorphism**.

We will further make use of two topological properties—connectedness and simple connectedness.

Definition 2.5. We say a matrix Lie group G is **connected** if for all A and B in G, there exists a path $A : [0,1] \to G$ such that $A(0) = A$ and $A(1) = B$.

This property is usually known as *path* connected, but matrix Lie groups are Lie groups (i.e., n-dimensional smooth manifolds) and therefore locally path connected. This means (by a standard result in topology) that for matrix Lie groups path connectedness is equivalent to connectedness (in the ordinary topological sense) and we are thus free to refer to them by the same name.

Even more important to our discussion is the notion of simple connectedness:

Definition 2.6. We say a matrix Lie group G is **simply connected** if it is connected and every closed path $A : [0,1] \to G$ is homotopically equivalent to a trivial path, i.e., there exists a continuous function $A(s,t)$ for $0 \leq s,t \leq 1$ in G such that:

1. $A(s,0) = A(s,1)$ for all s,
2. $A(0,t) = A(t)$,
3. $(A(1,t) = A(1,0)$ for all t.

As we shall see, the group SO(3) is not simply connected, but its universal cover, SU(2), is. The 2-1 homomorphism mentioned earlier has a kernel $\{I, -I\}$ corresponding to the fundamental group of SO(3). In fact SO(3) is isomorphic topologically to $\mathbb{RP}^3$ (S^3 with antipodal points identified) while SU(2) is isomorphic to S^3. The result is that there is a homotopically non-trivial path to the identity in SO(3), since in SU(2) this path corresponds to a path from I to $-I$.

2.2 Lie Algebras

Lie algebras, in the language of manifolds, are the tangent space at the identity to their respective Lie group. However, as we have foregone this language in favor of the language of matrices, we will give an alternate definition in terms of the **matrix exponential**. We define the exponential by generalizing the power series definition to matrices:

Definition 2.7. The **exponential** of an $n \times n$ matrix X, denoted e^X or $\exp(X)$ is defined by the power series

$$e^X = \sum_{m=0}^{\infty} \frac{X^m}{m!}$$

where X^0 is defined to be the identiy matrix I and X^m is the repeated matrix product of X with itself.

We list several useful properties of the matrix exponential.

Proposition 2.8. *Let X and Y be arbitrary $n \times n$ matrices. Then we have the following:*

1. $e^0 = I$.
2. $(e^X)^* = e^{X^*}$.
3. e^X *is invertible and* $(e^X)^{-1} = e^{-X}$.
4. $e^{(\alpha+\beta)X} = e^{\alpha X} e^{\beta X}$ *for all* α *and* β *in* $\mathbb{C}$.
5. *If* $XY = YX$*, then* $e^{X+Y} = e^X e^Y = e^Y e^X$.
6. *If* C *is in* $\mathrm{GL}(N;\mathbb{C})$*, then* $e^{CXC^{-1}} = Ce^X C^-1$.

Proof. See Chapter 2 of [1] □

Theorem 2.9. *For any $X \in M_n(\mathbb{C})$, we have*

$$\det(e^X) = e^{\mathrm{trace}(X)}.$$

Proof. If X is diagonalizable with eigenvalues $\lambda_1, \ldots, \lambda_n$, then e^X is diagonalizable with eigenvalues $e^{\lambda_1}, \ldots, e^{\lambda_n}$. Therefore $\mathrm{trace}(X) = \sum_j \lambda_j$ and

$$\det(e^X) = e^{\lambda_1} \ldots e^{\lambda_n} = e^{\lambda_1 + \ldots + \lambda_n} = e^{\mathrm{trace}(X)}.$$

This argument can be extended to a non-diagonalizable matrix X by approximating X with a sequence of diagonalizable matrices. □

Another important property of the exponential is the following:

Proposition 2.10. *Let X be an $n \times n$ complex matrix. Then e^{tX} is a smooth curve in $M_n(\mathbb{C})$ and*

$$\frac{d}{dt}e^{tX} = Xe^{tX} = e^{tX}X.$$

In particular,

$$\left.\frac{d}{dt}e^{tX}\right|_{t=0} = X.$$

Proof. See Chapter 2 of [1] □

Example 2.11. The matrix

$$X = \begin{pmatrix} 0 & -a \\ a & 0 \end{pmatrix}$$

has exponential

$$e^X = \begin{pmatrix} \cos a & -\sin a \\ \sin a & \cos a \end{pmatrix}$$

Proof. Note that the exponential of a diagonal matrix D with entries $\lambda_1, \ldots, \lambda_n$ is simply the diagonal matrix with entries $e^{\lambda_1}, \ldots, e^{\lambda_n}$. The eigenvectors of X are $(1, i)$ and $(i, 1)$ with eigenvalues $-ia$ and ia respectively. Therefore diagonalizing X and taking the exponential, we have

$$e^X = \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \begin{pmatrix} e^{-ia} & 0 \\ 0 & e^{ia} \end{pmatrix} \begin{pmatrix} 1/2 & -i/2 \\ -i/2 & 1/2 \end{pmatrix},$$

which simplifies to the claimed result. □

Already we can see similarities to angular momentum. Here a matrix X is defined as the derivative of an exponential, whereas in Section 1 we saw that the angular momentum operators could be thought of as the derivative of a rotation.

This connection will become even clearer with the Lie algebra of a matrix Lie group, which we now introduce. Although Lie algebras can be considered as abstract objects in their own right (e.g., $\mathbb{R}^3$ equipped with the cross product is a Lie algebra), we restrict our attention here to Lie algebras which are in some sense "matrix" Lie algebras—Lie algebras that are generated by matrix Lie groups or associated very closely with them.

Definition 2.12. Let $G \in M_n(\mathbb{C})$ be a matrix Lie group. We define the **Lie algebra** of G, denoted $\mathfrak{g}$, to be the set of all matrices $X \in M_n(\mathbb{C})$ such that e^{tX} is in G for all real numbers t.

Theorem 2.13. *Let G be a matrix Lie group with Lie algebra $\mathfrak{g}$. If X and Y are elements of $\mathfrak{g}$, then:*

1. $AXA^{-1} \in \mathfrak{g}$ *for all* $A \in G$.
2. $sX \in \mathfrak{g}$ *for all real numbers* s.
3. $X + Y \in \mathfrak{g}$
4. $XY - YX \in \mathfrak{g}$.

Proof. The first point follows simply from the properties of the matrix exponential:

$$e^{t(AXA^{-1})} = Ae^{tX}A^{-1} \in G$$

for all t. Furthermore for the second point, we simply note that $e^{t(sX)} = e^{(ts)X}$ is in G for all t since X is in $\mathfrak{g}$. For the third point, we use the **Lie product formula**:

$$e^{t(X+Y)} = \lim_{m\to\infty} \left(e^{tX/m}e^{tY/m}\right)^m.$$

The limit is invertible (since e^X is invertible for all X) and in G since G is a closed subgroup of $\mathrm{GL}(n, \mathbb{C})$. This holds for all t, so $X + Y \in \mathfrak{g}$.

The fourth point follows from points 2 and 3, which show that $\mathfrak{g}$ is a real subspace of $M_n(\mathbb{C})$ and therefore closed topologically, along with the following equality:

$$\begin{aligned} XY - YX &= \frac{d}{dt}\left(e^{tX}Ye^{-tX}\right)\Big|_{t=0} \\ &= \lim_{h\to 0} \frac{e^{hX}Ye^{-hX} - Y}{h} \end{aligned}$$

where the first equality follows from a straightforward application of the product rule. Together these imply that $XY - YX \in \mathfrak{g}$ since $e^{hX}Ye^{-hX}$ is in $\mathfrak{g}$ by point 1. □

For X and Y in $\mathfrak{g}$, we refer to $[X, Y] = XY - YX \in \mathfrak{g}$ as the **bracket** or **commutator** of X and Y. The gist of this theorem is that the Lie algebra is in fact a vector space equipped with a "bracket" operation (just as the space of linear operators in quantum mechanics has the commutator). Indeed this is how Lie algebras are defined abstractly, along with three additional properties on the bracket. We now prove these properties for the bracket we have defined.

Proposition 2.14. *Let G be a matrix Lie group with Lie algebra $\mathfrak{g}$. Then the bracket operation $[\cdot,\cdot] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ satisfies the following properties:*

1. $[\cdot,\cdot]$ *is bilinear,*
2. $[\cdot,\cdot]$ *is skew symmetric:* $[X,Y] = -[Y,X]$ *for all* $X, Y \in \mathfrak{g}$,
3. $[\cdot,\cdot]$ *satisfies the* ***Jacobi identity****:*

$$[X,[Y,Z]] + [Y,[Z,X]] + [Z,[X,Y]] = 0$$

for all X, Y, $Z \in \mathfrak{g}$.

Proof. The first two properties are obvious. We can verify the Jacobi identity by direct calculation:

$$\begin{aligned}[X,[Y,Z]] + [Y,[Z,X]] + [Z,[X,Y]] =& X(YZ - ZY) - (YZ - ZY)X + Y(ZX - XZ) \\ & - (ZX - XZ)Y + Z(XY - YX) - (YX - XY)Z \\ =& 0\end{aligned}$$

where the last equality follows by associativity of matrix multiplication. □

In analogy with Lie groups, we can define a Lie algebra homomorphism as a linear map that preserves the bracket operation between vector spaces.

Definition 2.15. Let $\mathfrak{g}$ and $\mathfrak{h}$ be Lie algebras. A linear map $\phi : \mathfrak{g} \to \mathfrak{h}$ is called a **Lie algebra homomorphism** if $\phi([X,Y]) = [\phi(X), \phi(Y)]$ for all $X, Y \in \mathfrak{g}$. If, in addition, ϕ is one-to-one and onto, then ϕ is called a **Lie algebra isomorphism**.

Lie algebra homomorphisms are associated Lie group homomorphisms by the following theorem:

Theorem 2.16. *Let* G *and* H *be matrix Lie groups with Lie algebras* $\mathfrak{g}$ *and* $\mathfrak{h}$ *respectively. Suppose that* $\Phi : G \to H$ *is a Lie group homomorphism. Then there exists a unique linear map* $\phi : \mathfrak{g} \to \mathfrak{h}$ *such that*

$$\Phi(e^X) = e^{\phi(X)} \tag{6}$$

for all $X \in \mathfrak{g}$. *In addition,* ϕ *satisfies the following properties:*

1. $\phi(AXA^{-1}) = \Phi(A)\phi(X)\Phi(A)^{-1}$ *for all* $X \in \mathfrak{g}$, $A \in G$.
2. $\phi([X,Y]) = [\phi(X), \phi(Y)]$ *for all* $X, Y \in \mathfrak{g}$ *(i.e.* ϕ *is a Lie algebra homomorphism)*
3. $\phi(X) = \frac{d}{dt}\Phi(e^{tX})\big|_{t=0}$ *for all* $X \in \mathfrak{g}$.

Proof. The proof requires a discussion of one-parameter subgroups, but it is otherwise similar to that of Theorem 2.13. See Chapter 3 of [1] for details. □

The most important takeaway of this theorem is that every Lie group homomorphism gives rise to a unique Lie algebra homomorphism associated with it. The converse, that every homomorphism of a Lie algebra $\mathfrak{g}$ corresponds to a homomorphism in the associated Lie group G, is only true if the group G is simply connected. As we shall see, this has important implications in the case of SO(3).

Finally in this subsection, we give a result that will be used shortly to prove a relationship between representations of Lie groups and Lie algebras.

Corollary 2.17. *If G is a connected matrix Lie group, then every element A of G may be written in the form*

$$A = e^{X_1} e^{X_2} \dots e^{X_m}$$

for some X_1, X_2, $\dots$, X_m in $\mathfrak{g}$.

Proof. See Chapter 2 of [**?**] □

2.3 Representations

We now move on to discussing Lie group and Lie algebra representations. The representations of SU(2), SO(3) and their Lie algebras play an important role in describing angular momentum and spin.

Definition 2.18. Let $G \in M_n(\mathbb{C})$ be a matrix Lie group and V be a finite-dimensional complex (real) vector space with $\dim(V) \geq 1$. A **finite-dimensional complex (real) representation** of G is a Lie group homomorphism

$$\Pi : G \to \mathrm{GL}(V).$$

If $\mathfrak{g}$ is a real or complex Lie algebra, then a **finite-dimensional complex (real) representation** of $\mathfrak{g}$ is a Lie algebra homomorphism

$$\pi : \mathfrak{g} \to \mathrm{gl}(V)$$

The following definition gives several relevant properties of representations and the spaces they act on.

Definition 2.19. Let Π be a finite-dimensional real or complex representation of a matrix Lie group G, acting on a space V. A subspace W of V is called **invariant** if $\Pi(A)w \in W$ for all $w \in W$ and all $A \in G$. An invariant subspace W is called **nontrivial** if $W \neq 0$ or V. A representation with no nontrivial invariant subspaces is called **irreducible**. These terms are defined analogously for Lie algebra representations.

We will elaborate more on the concept of representations in our discussion of SU(2) and SO(3). To finish the section we state the following important result:

Proposition 2.20. *Let G be a connected matrix Lie group with Lie algebra $\mathfrak{g}$.*

1. *If $\Pi : G \to \mathrm{GL}(V)$ is a representation of G and $\pi : \mathfrak{g} \to \mathrm{gl}(V)$ is the associated representation of $\mathfrak{g}$, then a subspace W of V is invariant under the action of G if and only if it is invariant under the action of $\mathfrak{g}$. In particular, Π is irreducible if and only if π is irreducible.*
2. *If Π_1 and Π_2 are representations of G and π_1 and π_2 are the associated Lie algebra representations, then π_1 and π_2 are isomorphic if and only if Π_1 and Π_2 are isomorphic.*

Proof. For Point 1, suppose first that $W \subset V$ is invariant under $\pi(X)$ for all $X \in \mathfrak{g}$. Now suppose A is an element of G. Since G is connected, Corollary 2.17 says that A can be written as $A = e^{X_1} \dots e^{X_m}$ for some $X_1, \dots, X_m \in \mathfrak{g}$. Since W is invariant under $\pi(X_j)$ it will also be invariant under $\exp(\pi(X_j)) = I + \pi(X_j) + \pi(X_j)^2/2 + \dots$ and, therefore, under

$$\begin{aligned} \Pi(A) = \Pi(e^{X_1} \dots e^{X_m}) &= \Pi(e^{X_1}) \dots \Pi(e^{X_m}) \\ &= e^{\pi(X_1)} \dots e^{\pi(X_m)}. \end{aligned}$$

Thus W is invariant under $\Pi(A)$ for all $A \in G$.

Conversely, suppose that W is invariant under $\Pi(A)$ for all $A \in G$. Then W is invariant under $\Pi(e^{tX})$ for all $X \in \mathfrak{g}$ and, hence, invariant under

$$\pi(X) = \frac{d}{dt}\Pi(e^{tX})\bigg|_{t=0}.$$

for all $X \in \mathfrak{g}$. This completes the proof of Point 1.

Now if Π_1 and Π_2 are two representations of G acting on vector spaces V_1 and V_2 respectively and $\Phi : V_1 \to V_2$ is an invertible linear map, then an argument similar to the one above shows that Φ is an isomorphism of group representations if and only if it is an isomorphism of Lie algebra representations. □

This result ensures that our future discussion of SU(2) and SO(3) will be useful. Rotations can be thought of as a Lie group representation, while angular momentum is the associated Lie algebra representation. Without Proposition 2.20, we would have no guarantee that the irreducible representations of a group are uniquely associated with irreducible representations of the Lie algebra, and thus any attempt to relate angular momentum to rotations would run into the danger of not being well-defined.

3 SU(2) and SO(3)

3.1 Definitions and Properties

We now move on to our discussion of SU(2) and SO(3). We begin by defining the group SU(n) and stating some important results for SU(2).

Definition 3.1. An $n \times n$ complex matrix A is said to be **unitary** if the column vectors of A are orthonormal, that is, if

$$\sum_{l=1}^{n} \overline{A_{lj}} A_{kl} = \delta_{jk}, \tag{7}$$

where δ_{jk} is the Kronecker delta, equal to 1 if $j = k$ and equal to 0 otherwise. The collection of $n \times n$ unitary matrices is a closed subgroup of GL(n; $\mathbb{C}$), which we call the **unitary group** of order n and denote by U(n). The subgroup of U(n) consisting of unitary matrices with determinant one is called the **special unitary group** of order n and denoted SU(n).

We will not include the proof that U(n) and SU(n) are matrix Lie groups, as it is a relatively straightforward computation. The group SU(n) may be thought of as 'rotations' on $\mathbb{C}^n$.

Two equivalent definitions of a unitary matrix A are (1) the adjoint matrix of A is the inverse of A (i.e., $A^* = A^{-1}$) and (2) A preserves the standard inner product $\langle \cdot, \cdot \rangle$ on $\mathbb{C}^n$, defined by

$$\langle \mathbf{x}, \mathbf{y} \rangle = \sum_j \overline{x_j} y_j.$$

By 'preserves' we mean $\langle A\mathbf{x}, A\mathbf{y} \rangle = \langle \mathbf{x}, \mathbf{y} \rangle$ for all $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$. To see that these definitions are equivalent to the one given above, first note that we may rewrite equation (7) as

$$\sum_{l=1}^{n} (A^*)_{jl} A_{kl} = \delta_{jk},$$

which says that $A^*A = I$. Thus A is unitary if and only if $A^* = A^{-1}$ (note that this follows only in the finite-dimensional case). Meanwhile, standard properties of the adjoint say that

$$\langle \mathbf{x}, A\mathbf{y} \rangle = \langle A^*\mathbf{x}, \mathbf{y} \rangle$$

for all $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$. Therefore if A is unitary,

$$\langle A\mathbf{x}, A\mathbf{y} \rangle = \langle A^*A\mathbf{x}, \mathbf{y} \rangle = \langle I\mathbf{x}, \mathbf{y} \rangle = \langle \mathbf{x}, \mathbf{y} \rangle,$$

showing that A preserves the inner product. On the other hand, if A preserves the inner product, then $\langle A^*A\mathbf{x}, \mathbf{y}\rangle = \langle \mathbf{x}, \mathbf{y}\rangle$ for all $\mathbf{x}, \mathbf{y}$. By letting $\mathbf{y}$ range over the standard basis vectors, it is easy to see that this condition holds only if $A^*A = I$.

A further property of unitary matrices comes from the fact that $\det A^* = \overline{\det A}$ for any matrix A. Thus, if A is unitary, we have

$$\det(A^*A) = |\det A|^2 = \det I = 1.$$

So all unitary matrices have determinant with magnitude 1.

The group SU(2) is of special importance. We now describe its structure and give the form of its Lie algebra.

Proposition 3.2. *Elements of* SU(2) *can be uniquely expressed in the form*

$$U = \begin{pmatrix} \alpha & -\overline{\beta} \\ \beta & \overline{\alpha} \end{pmatrix}$$

where α and β are elements of $\mathbb{C}$ satisfying $|\alpha|^2 + |\beta|^2 = 1$.

Proof. Let $U \in \mathrm{SU}(2)$. Clearly the first column of U,

$$\mathbf{v}_1 = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

must take such a form, so we merely need to show that the second column is exactly determined by the first. The second column must be orthogonal to the first and be a unit vector. One such vector is

$$\mathbf{v}_2 = \begin{pmatrix} -\overline{\beta} \\ \overline{\alpha} \end{pmatrix},$$

but $\mathbf{v}_1$ and $\mathbf{v}_2$ span $\mathbb{C}^2$, so every unit vector orthogonal to $\mathbf{v}_1$ must be of the form $e^{i\theta}\mathbf{v}_2$. Therefore any element of SU(2) takes the form

$$U = \begin{pmatrix} \alpha & -e^{i\theta}\overline{\beta} \\ \beta & e^{i\theta}\overline{\alpha} \end{pmatrix}.$$

However we have left out one property of U, namely that $\det(A) = 1$. The above matrix has determinant $e^{i\theta}(|\alpha|^2 + |\beta|^2) = e^{i\theta}$, so we require that $e^{i\theta} = 1$. This implies

$$U = \begin{pmatrix} \alpha & -\overline{\beta} \\ \beta & \overline{\alpha} \end{pmatrix}.$$

as desired. □

Corollary 3.3. SU(2) *is simply connected.*

Proof. Elements of SU(2) are completely defined by the α and β given in Proposition 3.2. Therefore we can think of SU(2) topologically as S^3, which is simply connected. □

Proposition 3.4. *The Lie algebra of* U(n)*, denoted* u(n)*, consists of all $n \times n$ skew self-adjoint complex matrices, i.e., matrices satisfying $X^* = -X$. The Lie algebra of* SU(n)*, denoted* su(n)*, consists of all $n \times n$ skew self-adjoint complex matrices such that* trace$(X) = 0$*. In particular* su(2)*, the Lie algebra of* SU(2)*, consists of matrices of the form*

$$X = \begin{pmatrix} ai & -b+ci \\ b+ci & -ai \end{pmatrix}$$

for a, b, c elements of $\mathbb{R}$*.*

Proof. A matrix U is unitary if and only if $U^* = U^{-1}$. Therefore for any matrix X, $e^{tX} \in \mathrm{U}(n)$ if and only if

$$(e^{tX})^* = (e^{tX})^{-1} = e^{-tX}.$$

But $(e^{tX})^* = e^{tX^*}$, so in fact $e^{tX} \in \mathrm{U}(n)$ if and only if

$$e^{tX^*} = e^{-tX}.$$

Clearly if X is skew self-adjoint then this condition holds and so X is in u(n). Conversely, we know that if X is in the Lie algebra, then the condition holds and we may write

$$X^* = \frac{d}{dt}(e^{tX^*})\bigg|_{t=0} = \frac{d}{dt}(e^{-tX})\bigg|_{t=0} = -X$$

proving the first part of the proposition.

Now if X has trace zero, then e^{tX} has determinant one for all t by , which implies $X \in \mathrm{su}(n)$. On the other hand if e^{tX} has determinant one for all t, then

$$\mathrm{trace}(X) = \frac{d}{dt} e^{t\mathrm{trace}(X)}\bigg|_{t=0} = 0,$$

proving that su(n) consists of skew self-adjoint matrices with trace zero. In particular, this implies that elements of su(2) take the form

$$X = \begin{pmatrix} ai & -b+ci \\ b+ci & -ai \end{pmatrix}$$

for a, b, c elements of $\mathbb{R}$. □

Next we define SO(n) and discuss properties of SO(3).

Definition 3.5. An $n \times n$ real matrix A is said to be **orthogonal** if the column vectors of A are orthonormal

The collection of $n \times n$ orthogonal matrices is a closed subgroup of $\mathrm{GL}(n;\mathbb{C})$ which we call the **orthogonal group** of order n and denote by O(n). The subgroup of O(n) consisting of orthogonal matrices with determinant one is called the **special orthogonal group** of order n and denoted SO(n).

SO(n) may be thought of as the space of rotations on $\mathbb{R}^n$. We will not prove that O(n) is a Lie group and leave it as an exercise for the reader. As with unitarity, we have two equivalent definitions for orthogonality. They are (1) the transpose of A equals its inverse (i.e., $A^{tr} = A^{-1}$) and (2) A preserves the inner product on $\mathbb{R}^n$.

In analogy with U(n), we find that the determinant of an orthogonal matrix A must have magnitude 1. But this time the determinant must also be real (since A is real), so $\det A = \pm 1$. This property is important for the following proposition.

Proposition 3.6. O(n) *is not connected for all n.*

Proof. The determinant is a continuous map from $M_n(\mathbb{C})$ to $\mathbb{C}$. In particular, its restriction to real matrices is a continuous map into $\mathbb{R}$, and so the image of any connected subset of $M_n(\mathbb{R})$ must be a connected set in $\mathbb{R}$. But we have just argued that the image of O(n) is $\{1, -1\}$ which is not connected. Thus O(n) is not a connected subset of $M_n(\mathbb{R})$. □

On the other hand, by definition the image of the determinant for SO(n) is $\{1\}$. We will prove later that SO(3) is homeomorphic to 3-dimensional real projective space, which is connected but not simply connected.

Proposition 3.7. *Elements of* SO(3) *are rotations in* $\mathbb{R}^3$*, i.e., an element R of* SO(3) *can be expressed in the form*

$$R = R_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta) & -\sin(\theta) \\ 0 & \sin(\theta) & \cos(\theta) \end{pmatrix} R_0^{-1}$$

for $\theta \in [0, 2\pi)$ *and* R_0 *an element of* SO(3).

Proof. We first show that R has an eigenvector v with eigenvalue 1. Note that because R is an element of SO(3), it is also an element of SU(3), and so every (real or complex) eigenvalue of R must have absolute value 1. This is because if there existed an eigenvector $\mathbf{v} \in \mathbb{C}^3$ with eigenvalue λ such that $|\lambda|^2 \neq 1$, then we would have

$$\langle R\mathbf{v}, R\mathbf{v}\rangle = \langle \lambda\mathbf{v}, \lambda\mathbf{v}\rangle = |\lambda|^2\langle \mathbf{v}, \mathbf{v}\rangle \geq \langle \mathbf{v}, \mathbf{v}\rangle,$$

contradicting that R is an element of SU(3).

Furthermore R is a real matrix, so its eigenvalues come in conjugate pairs. R has precisely three eigenvalues (because R is normal), so it must have at least one that is real and two that are conjugates of each other. We denote the real eigenvalue by λ and the conjugate eigenvalues by μ and $\overline{\mu}$ (it is possible that μ and $\overline{\mu}$ are also real, in which case they are both 1 or -1).

Finally, because $R \in \mathrm{SO}(3)$ we require that $\det(R) = 1$. But because each eigenvalue has magnitude 1, $\det(R) = \lambda\mu\overline{\mu} = \lambda|\mu|^2 = \lambda$, so $\mathbf{v}$ is an eigenvector of R with eigenvalue $\lambda = 1$ as desired.

Next we show that the orthogonal complement of $\mathbf{v}$ in $\mathbb{R}^3$ is an invariant subspace of R, i.e., R maps the plane orthogonal to $\mathbf{v}$ into itself. Let $\mathbf{w}$ be an element of $\mathbf{v}^{\perp}$. Then $\langle \mathbf{v}, \mathbf{w}\rangle = 0$, so

$$\langle \mathbf{v}, R\mathbf{w}\rangle = \langle R^{-1}\mathbf{v}, \mathbf{w}\rangle = \frac{1}{\lambda}\langle v, w\rangle = 0$$

showing that $R\mathbf{w}$ is also in $\mathbf{v}^{\perp}$. Thus R leaves the span of $\mathbf{v}$ untouched while acting on $\mathbf{v}^{\perp}$. In other words, R is similar to a matrix of the form

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & a & b \\ 0 & c & d \end{pmatrix} \tag{8}$$

for $a, b, c, d \in \mathbb{R}$. Moreover we can easily choose an oriented orthonormal basis with first element $\mathbf{v}$, so that the change of basis matrix R_0 will be orthogonal with determinant 1. To determine the values of a, b, c, and d, first note that the columns in (8) must be orthonormal, so the middle column may be written

$$\begin{pmatrix} 0 \\ \cos(\theta) \\ \sin(\theta) \end{pmatrix}$$

for some $\theta \in [0, 2\pi]$. The third column can be expressed similarly, but must also be orthogonal to the second column, which implies it is either

$$\begin{pmatrix} 0 \\ -\sin(\theta) \\ \cos(\theta) \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 0 \\ \sin(\theta) \\ -\cos(\theta) \end{pmatrix}.$$

Only the first possibility results in a matrix with determinant 1, so we conclude that R may be expressed

$$R = R_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta) & -\sin(\theta) \\ 0 & \sin(\theta) & \cos(\theta) \end{pmatrix} R_0^{-1}$$

as desired. □

Proposition 3.8. *The Lie algebra of* $\mathrm{O}(n)$ *is equal to the Lie algebra of* $\mathrm{SO}(n)$ *and consists of all* $n \times n$ *real matrices satisfying* $X^{tr} = -X$. *We denote this Lie algebra by* $\mathrm{so}(n)$. *In particular* $\mathrm{so}(3)$, *the Lie algebra of* $\mathrm{SO}(3)$, *consists of matrices of the form*

$$X = \begin{pmatrix} 0 & a & b \\ -a & 0 & c \\ -b & -c & 0 \end{pmatrix}$$

for a, b, c *elements of* $\mathbb{R}$.

Proof. We can apply the same argument as that used in the proof of Proposition 3.4 but restricted to the reals. In this case the adjoint becomes the transpose, and so the condition on the Lie algebra $\mathrm{o}(n)$ becomes $X^{tr} = -X$. However this condition implies $\mathrm{trace}(X) = 0$, so in fact every element of $\mathrm{o}(n)$ is also an element of $\mathrm{so}(n)$.

For the three-dimensional case, the condition $X^{tr} = -X$ implies that the diagonal entries of X are zero and opposing terms are the minus of each other, so that X takes the form

$$X = \begin{pmatrix} 0 & a & b \\ -a & 0 & c \\ -b & -c & 0 \end{pmatrix}, \quad a, b, c \in \mathbb{R}$$

as desired. □

Proposition 3.9. *The Lie algebras of* $\mathrm{SU}(2)$ *and* $\mathrm{SO}(3)$ *are isomorphic.*

Proof. The Lie algebra $\mathrm{su}(2)$ has a basis

$$E_1 = \frac{1}{2}\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}, \quad E_2 = \frac{1}{2}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad E_3 = \frac{1}{2}\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$$

with commutation relations $[E_1, E_2] = E_3$, $[E_2, E_3] = E_1$, and $[E_3, E_1] = E_2$. Similarly the Lie algebra $\mathrm{so}(3)$ has a basis

$$F_1 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad F_2 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad F_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix},$$

with commutation relations $[F_1, F_2] = F_3$, $[F_2, F_3] = F_1$, and $[F_3, F_1] = F_2$. By skew symmetry, these relations completely determine the bracket operation on the bases for su(2) and so(3), and therefore on the spaces themselves. Thus because the bases satisfy the same commutation relations, the brackets on the two Lie algebras are the same. Hence su(2) and so(3) are isomorphic as Lie algebras. □

Physicists will recognize the basis for su(2) as the Pauli spin matrices multiplied by a factor of i. Clearly spin and the Lie algebra su(2) are closely related, but the precise connection requires a classification of the representations of su(2) to fully understand. This calculation will be performed in Section 5.

3.2 2-1 Homomorphism

We now make the connection between SU(2) and SO(3) explicit by constructing a 2-1 homomorphism between the two. First we define a Lie group representation (and its associated Lie algebra representation) which will be useful in the construction.

Definition 3.10. Let G be a matrix Lie group with Lie algebra $\mathfrak{g}$. Then for each $A \in G$, we define the **adjoint map** of G as a linear map $\mathrm{Ad}_A : \mathfrak{g} \to \mathfrak{g}$ by the formula

$$\mathrm{Ad}_A(X) = AXA^{-1}. \tag{9}$$

Proposition 3.11. *The map* $\mathrm{Ad} : G \to \mathrm{GL}(\mathfrak{g})$ *defined by* $A \mapsto \mathrm{Ad}_A$ *is a representation of* G *acting on* $\mathfrak{g}$*. Furthermore, for each* $A \in G$*,* Ad_A *satisfies* $\mathrm{Ad}_A([X, Y]) = [\mathrm{Ad}_A(X), \mathrm{Ad}_A(Y)]$ *for all* $X, Y \in \mathfrak{g}$*.*

Proof. $\mathrm{Ad}_A(X)$ is in $\mathfrak{g}$ by Point 1 of Theorem 2.13. That Ad_A is a homomorphism and $\mathrm{Ad}_A([X, Y]) = [\mathrm{Ad}_A(X), \mathrm{Ad}_A(Y)]$ can both be seen immediately from the definition. □

Proposition 3.12. *Let* $\mathrm{ad} : \mathfrak{g} \to \mathrm{gl}(\mathfrak{g})$ *be the representation of* $\mathfrak{g}$ *associated to* Ad *as defined in equation (9). Then for all* $X, Y \in \mathfrak{g}$*,*

$$\mathrm{ad}_X(Y) = [X, Y].$$

Proof. By Point 3 of Theorem 2.16, ad can be computed as

$$\mathrm{ad}_X = \frac{d}{dt}\mathrm{Ad}_{e^{tX}}\bigg|_{t=0},$$

which gives

$$\mathrm{ad}_X(Y) = \frac{d}{dt}e^{tX}Ye^{-tX}\bigg|_{t=0} = [X, Y]$$

as desired. □

The construction of the 2-1 and onto homomorphism of SU(2) into SO(3) is as follows. Consider the adjoint map $\Phi = \mathrm{Ad}$ for $G = \mathrm{SU}(2)$. Then as noted above, $\mathfrak{g} = \mathrm{su}(2)$ is the collection of all complex 2×2 matrices X satisfying $X^* = -X$ and $\mathrm{trace}(X) = 0$. i.e., matrices of the form

$$X = i \begin{pmatrix} x_1 & x_2 + ix_3 \\ x_2 - ix_3 & -x_1 \end{pmatrix},$$

for $x_1, x_2, x_3 \in \mathbb{R}$. We can thus identify $\mathfrak{g}$ with $\mathbb{R}^3$ via the coordinates x_1, x_2, and x_3, and then the standard inner product on $\mathbb{R}^3$ (the dot product) may be written as

$$\langle X_1, X_2 \rangle = -\frac{1}{2}\mathrm{trace}(X_1 X_2).$$

That is to say,

$$-\frac{1}{2}\mathrm{trace}\left(i \begin{pmatrix} x_1 & x_2 + ix_3 \\ x_2 - ix_3 & -x_1 \end{pmatrix} i \begin{pmatrix} x_1' & x_2' + ix_3' \\ x_2' - ix_3' & -x_1' \end{pmatrix} \right) = x_1x_1' + x_2x_2' + x_3x_3'$$

as may be easily verified by direct calculation.

Viewed in this way, we can think of $\Phi_U = \mathrm{Ad}_U$ as a linear map on $\mathbb{R}^3$ for each $U \in \mathrm{SU}(2)$. The map is clearly well-defined by Theorem 2.13 part (1), and moreover

$$\begin{aligned} -\frac{1}{2}\mathrm{trace}(\Phi_U(X_1)\Phi_U(X_2)) &= -\frac{1}{2}\mathrm{trace}((UX_1U^{-1})(UX_2U^{-1})) \\ &= -\frac{1}{2}\mathrm{trace}(UX_1X_2U^{-1}) \\ &= -\frac{1}{2}\mathrm{trace}(X_1X_2) \end{aligned}$$

(since the trace is invariant under conjugation), showing that Φ_U preserves the inner product $-\mathrm{trace}(X_1X_2)/2$ on $\mathrm{su}(2) \cong \mathbb{R}^3$. Therefore $\Phi = \mathrm{Ad}$ is actually a Lie group homomorphism of SU(2) into the group of orthogonal linear transformations of $\mathbb{R}^3$, i.e., into O(3). But SU(2) is connected and Φ is continuous (as it is a Lie group homomorphism), so Φ_U lies in the identity component of O(3). Because $\det I = 1$, every element of the identity component must have determinant 1 (otherwise it would not be connected) and thus Φ_U lies in SO(3). Therefore Φ is in fact a homomorphism of SU(2) into SO(3).

For example, suppose U is the matrix

$$U = \begin{pmatrix} e^{i\theta/2} & 0 \\ 0 & e^{-i\theta/2} \end{pmatrix}. \tag{10}$$

Then for X defined as above,

$$Ui\begin{pmatrix} x_1 & x_2+ix_3 \\ x_2-ix_3 & -x_1 \end{pmatrix}U^{-1} = i\begin{pmatrix} x_1' & x_2'+ix_3' \\ x_2'-ix_3' & -x_1' \end{pmatrix}, \tag{11}$$

where $x_1' = x_1$ and

$$\begin{aligned} x_2' + ix_3' &= e^{i\theta}(x_2+ix_3) \\ &= (x_2\cos\theta - x_3\sin\theta) + i(x_2\sin\theta + x_3\cos\theta). \end{aligned} \tag{12}$$

So $\Phi = \mathrm{Ad}_U$ is a rotation by angle θ in the $(x_2, x_3)-$plane. Surprisingly, the rotation is by θ and not by $\theta/2$. This observation will come into play later when we discuss spin angular momentum (it is behind the unusual behavior of spin-1/2 particles).

Proposition 3.13. *The map $U \mapsto \Phi_U$ is a 2-1 and onto homomorphism of* SU(2) *to* SO(3) *with kernel equal to $\{I, -I\}$.*

Proof. We first show that the kernel of Φ is $\{I, -I\}$, and hence that Φ is 2-1. Both I and $-I$ are clearly elements of the kernel, as they commute through the conjugation. To see that these are the only elements in $\ker(\Phi)$, let U be an element of $\ker(\Phi)$, which we may express as

$$U = \begin{pmatrix} \alpha & -\overline{\beta} \\ \beta & \overline{\alpha} \end{pmatrix}$$

by Proposition 3.2. Then $\Phi_U(X) = UXU^{-1} = X$ for all $X \in \mathrm{su}(2)$, which implies that U commutes with every element of su(2). Note that this implies U also commutes with scalar multiples of su(2), and in particular matrices of the form

$$-iX = \begin{pmatrix} x_1 & x_2+ix_3 \\ x_2-ix_3 & -x_1 \end{pmatrix},$$

which can be obtained by multiplying elements of su(2) by $-i$. Thus if

$$X = i\begin{pmatrix} x_1 & x_2+ix_3 \\ x_2-ix_3 & -x_1 \end{pmatrix}, \quad Y = i\begin{pmatrix} y_1 & y_2+iy_3 \\ y_2-ix_3 & -x_1 \end{pmatrix}$$

are arbitrary elements of su(2), then U commutes with

$$\begin{pmatrix} a & b \\ c & -a \end{pmatrix} = X + iY, \tag{13}$$

where a, b, and c are arbitrary complex numbers. Furthermore, U commutes with scalar multiples of the identity kI for $k \in \mathbb{C}$, and adding this to equation (13) gives matrices of the form

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad a, b, c, d \in \mathbb{C}.$$

In other words, U commutes with every element of $M_2(\mathbb{C})$. But this implies U must be either I or $-I$, for if it commutes with every matrix then it commutes as follows:

$$\begin{pmatrix} \alpha & -\overline{\beta} \\ \beta & \overline{\alpha} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \alpha & -\overline{\beta} \\ \beta & \overline{\alpha} \end{pmatrix},$$

$$\begin{pmatrix} \alpha & -\overline{\beta} \\ \beta & \overline{\alpha} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \alpha & -\overline{\beta} \\ \beta & \overline{\alpha} \end{pmatrix}.$$

The first equation implies that $\alpha = \overline{\alpha}$ and the second implies that $\beta = -\overline{\beta} = 0$. Together these give us that $\alpha = \pm 1$ (since $|\alpha|^2 + |\beta|^2 = 1$). This completes the proof that $\ker(\Phi) = \{I, -I\}$.

To show that Φ maps *onto* SO(3), let R be an element of SO(3). We want to show that R can be expressed as $\Phi(U) = Ad_U$ for some $U \in SU(2)$. But by Proposition 3.7, we can express R as a rotation by angle θ around an "axis" $X \in \mathfrak{g} \cong \mathbb{R}^3$. Because X is an element of $\mathfrak{g} = \mathrm{su}(2)$, it is skew self-adjoint, and therefore by the Spectral Theorem we may write

$$X = iU_0 \begin{pmatrix} x_1 & 0 \\ 0 & -x_1 \end{pmatrix} U_0^{-1},$$

where U_0 is a 2×2 unitary matrix. Then the plane orthogonal to X in $\mathfrak{g}$ is the space of matrices of the form

$$X' = iU_0 \begin{pmatrix} 0 & x_2 + ix_3 \\ x_2 - ix_3 & 0 \end{pmatrix} U_0^{-1}. \tag{14}$$

Now if we let

$$U = U_0 \begin{pmatrix} e^{i\theta/2} & 0 \\ 0 & e^{-i\theta/2} \end{pmatrix} U_0^{-1},$$

then it is easy to see that UXU^{-1}. On the other hand, the calculations given in equations (11) and (12) show that $UX'U^{-1}$ is of the same form as in equation (14), but with (x_2, x_3) rotated by angle θ. Therefore Φ_U is a rotation by angle θ in the plane perpendicular to X, showing that Φ_U coincides with R. In other words, Φ maps onto every element of SO(3). $\square$

Because SU(2) is homeomorphic to S^3, Proposition 3.13 implies that SO(3) is homeomorphic to S^3 with antipodal points identified, which is the space commonly known as $\mathbb{RP}^3$, or 3-dimensional real projective space. $\mathbb{RP}^3$ is connected but not simply connected, so we have the following corollary:

Corollary 3.14. SO(3) *is connected but not simply connected.*

We have already shown that the Lie algebras su(2) and so(3) are isomorphic. Given that Proposition 3.13 proves that SU(2) and SO(3) are *not* isomorphic, we can surmise that something fishy is going on.

The perspective of manifolds offers an explanation for the discrepancy. The Lie algebra of a Lie group is the tangent space at the identity, so it captures the local behavior of the group. Thus it makes sense that su(2) and so(3) should be isomorphic, because the Lie groups are at least 'locally' isomorphic (as the 2-1 homomorphism shows). But in converting from Lie group to Lie algebra, some information is lost, and this is enough to let the 2-1 homomorphism descend to an isomorphism of the Lie algebras. The information loss is of further importance when classifying representations of the Lie groups and Lie algebras. This is the topic of the next section.

4 Classifying Irreducible Representations

Thus far we have only seen hints of how angular momentum relates to the groups SU(2) and SO(3), and to their Lie algebra su(2) $\cong$ so(3). The connection will become more clear in this section, though the final fruits of our labor will have to wait for Section 5. But to give a preview: the angular momentum operators L_1, L_2, and L_3 form a representation of so(3) on the space of three-dimensional wavefunctions, i.e., on $L^2(\mathbb{R}^3)$. This representation is associated to a representation Π of SO(3), which is the natural action of the rotation group on the space of wavefunctions:

$$(\Pi(R)\psi)(\mathbf{x}) = \psi(R^{-1}\mathbf{x})$$

for R an element of SO(3). It turns out that these representations are "completely reducible" to irreducible representations of so(3) and SO(3) which act on finite dimensional vector spaces of $L^2(\mathbb{R}^3)$. Thus by classifying the irreducible representations, we are able to fully describe the invariant subspaces of the angular momentum operators, and therefore able to fully describe the solutions of the rotationally invariant Schrödinger equation.

4.1 The Irreducible Representations of so(3)

We begin with the irreducible representations of so(3). The analysis we now perform should be instantly recognizable to any student of quantum mechanics as the computation of the eigenvalues of the angular momentum operators (cf. [3] pp. 145-49 and [4] pp. 168-171).

Theorem 4.1. *For each $l = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$ there exists an irreducible representation of* so(3) *of dimension $2l+1$. Furthermore, any two irreducible representations of* so(3) *with the same dimension are isomorphic.*

Note that because $2l+1$ ranges over all positive integers, l completely determines the irreducible representations of so(3) $\cong$ su(2). For each l there is exactly one irreducible representation (of dimension $2l+1$), and for each irreducible representation there is a corresponding l.

Proof. Let π be an irreducible representation of so(3) acting on a finite-dimensional vector space V. We begin by defining operators L_1, L_2, and L_3 on V by

$$L_1 = i\pi(F_1), \quad L_2 = i\pi(F_2), \quad \text{and} \quad L_3 = i\pi(F_3) \tag{15}$$

where F_1, F_2, and F_3 are the basis elements for so(3) defined in the proof of Proposition 3.9. Because π is a Lie algebra homomorphism, the L_j's satisfy the same commutation relations as the F_j's, so we have

$$[L_1, L_2] = iL_3; \quad [L_2, L_3] = iL_1; \quad [L_3, L_1] = iL_2;$$

which we see are precisely the same commutation relations as those found for the angular momentum operators in equation (4) without a factor of $\hbar$. Thus we can think of L_1, L_2, and L_3 as the *dimensionless* angular momentum operators.

Next we define two new operators L_+ and L_- as linear combinations of L_1 and L_2:

$$\begin{aligned} L_+ &= i\pi(F_1) - \pi(F_2) = L_1 + iL_2 \\ L_- &= i\pi(F_1) + \pi(F_2) = L_1 - iL_2 \end{aligned}$$

Then it is easy to check that L_+, L_-, and L_3 satisfy the commutation relations

$$\begin{aligned} [L_3, L_+] &= L_+ \\ [L_3, L_-] &= -L_- \\ [L_+, L_-] &= 2L_3. \end{aligned} \tag{16}$$

We have the following lemma relating the eigenvectors of these three operators:

Lemma 4.2. *Let u be an eigenvector of L_3 with eigenvalue $\alpha \in \mathbb{C}$. Then we have*

$$L_3 L_+ u = (\alpha + 1) L_+ u.$$

Thus, either $L_+ u = 0$ or $L_+ u$ is an eigenvector for L_3 with eigenvalue $\alpha + 1$. Similarly,

$$L_3 L_- u = (\alpha - 1) L_- u,$$

so that either $L_- u = 0$ or $L_- u$ is an eigenvector for L_3 with eigenvalue $\alpha - 1$.

In quantum mechanics, L_+ is known as the "raising operator" and L_- is known as the "lowering operator" for obvious reasons.

Proof of Lemma. We know that

$$[L_3, L_+] = [i\pi(F_3), i\pi(F_1) - \pi(F_2)] = \pi([iF_3, iF_1 - F_2]) = L_+.$$

Thus we have,

$$\begin{aligned} L_3 L_+ u &= L_+ L_3 u + L_+ u \\ &= L_+(\alpha u) + L_+ u \\ &= (\alpha + 1) L_+ u. \end{aligned}$$

Replacing L_+ with L_- in the argument above gives the second half of the lemma. □

We now return to the proof of the theorem. Since we are working over the algebraically closed field $\mathbb{C}$, the operator L_3 must have at least one eigenvector u with eigenvalue α. Applying Lemma 4.2 repeatedly, we find eigenvectors for L_3 with eigenvalues increasing by 1 at each step:

$$L_3 (L_+)^k u = (\alpha + k)(L_+)^k u.$$

Since these eigenvectors have distinct eigenvalues, they are linearly independent. Therefore at some point the series must terminate, because V is a finite-dimensional vector space. Thus there is some $N \geq 0$ such that

$$(L_+)^N u \neq 0$$

but

$$(L_+)^{N+1} = 0.$$

We now define $u_0 := (L_+)^N u$ and $\lambda := \alpha + 2N$. Then u_0 is a non-zero vector with

$$\begin{aligned} L_+ u_0 &= 0 \\ L_3 u_0 &= \lambda u_0. \end{aligned}$$

Forgetting about the original eigenvector u and eigenvalue α we define vectors

$$u_k = (L_-)^k u_0$$

for $k \geq 0$, which by Lemma 4.2 are all eigenvectors of L_3 with eigenvalues $\lambda - k$:

$$L_3 u_k = (\lambda - k) u_k.$$

Again this gives a series of linearly independent eigenvectors of L_3, so again the series must terminate, i.e., there is some integer $M \geq 0$ such that

$$u_k = (L_-)^k u_0 \neq 0$$

for all $k \leq M$, but

$$u_{M+1} = (L_-)^{M+1} u_0 = 0.$$

We have now discovered a chain of eigenvectors for L_3 defined by the two numbers M and λ. We are able to relate these values to each other using the following lemma:

Lemma 4.3. *For u_k defined as in equation (4.1) and $k \geq 1$, we have*

$$L_+ u_k = k[2\lambda - (k-1)] u_{k-1} \tag{17}$$

Proof of Lemma. We proceed by induction on k. The commutation relation given in equation (16) implies $L_+ L_- = 2L_3 + L_- L_+$, so by the definition of the u_k's in terms of u_0,

$$L_+ u_1 = L_+ L_- u_0 = (2L_3 + L_- L_+) u_0 = 2\lambda u_0 + L_- 0 = 2\lambda u_0,$$

which verifies equation (17) in the case $k = 1$. Now assume equation (17) holds for some $k \geq 1$. Again using equation (16) and writing u_{k+1} in terms of u_k, we find,

$$\begin{aligned} L_+ u_{k+1} &= L_+ L_- u_k \\ &= (2L_3 + L_- L_+) u_k \\ &= 2(\lambda - k) u_k + k[2\lambda - (k-1)] L_- u_{k-1} \\ &= (k+1)[2\lambda - ((k+1) - 1)] u_k, \end{aligned}$$

which is equation (17) for $k+1$. Therefore the formula holds for all $k \geq 1$. □

Now because $u_{M+1} = 0$, we must have $L_+ u_{M+1} = 0$. Hence by (17),

$$0 = L_+ u_{M+1} = (M+1)(2\lambda - M)u_M.$$

But u_M and $M+1$ are both nonzero, so we must have that $2\lambda - M = 0$, i.e., $\lambda = M/2$. We define $l = \lambda = M/2$, so that the largest eigenvalue of L_3 is just the value l. Therefore for every irreducible representation (π, V) of so(3), there exists a number $l = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$ and nonzero vectors $u_0, \dots u_{2l}$ such that

$$\begin{aligned} L_3 u_k &= (l-k)u_k \\ L_- u_k &= \begin{cases} u_{k+1} & k \leq 2l \\ 0 & k = 2l \end{cases} \\ L_+ u_k &= \begin{cases} k(2l-(k-1))u_{k-1} & k \geq 0 \\ 0 & k = 0 \end{cases} \end{aligned} \tag{18}$$

In quantum mechanics the value l is known as the **spin** of the representation (π, V) of so(3). As mentioned above, the vectors $u_0, \dots u_{2l}$ are linearly independent. Moreover, their span is an invariant subspace under the L_3, L_+, and L_- operators, hence under L_1, L_2 and L_3, and hence under every action of so(3) on V (since every action of so(3) is a complex linear combination of the L_j's). But the span is not $\{0\}$ since it contains the nonzero vector u_0, so because π is an irreducible representation, $u_0, \dots u_{2l}$ must span all of V.

This proves that every irreducible representation of so(3) is of the form (18) for some $l = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$, which implies that any two irreducible representations with the same dimension (equal to $2l+1$) must be isomorphic. It remains to show that such a representation exists for every value of l.

To do this, we *define* a vector space V with basis $u_0, u_1, \dots, u_{2l}$, and then define the action of so(3) via (18). This completely defines the action because any action of so(3) can be constructed as a linear combination of L_+, L_-, and L_3. To see that (π, V), defined in this way, is indeed a representation of so(3), we merely need to show that L_+, L_-, and L_3 satisfy the commutation relations given in (16).

To this end, consider the action of $[L_3, L_+]$ on a basis element u_k. If $k = 0$, then

$$[L_3, L_+]u_0 = (L_3 L_+ - L_+ L_3)u_0 = L_3 0 - l L_+ u_0 = 0 = L_+ u_0,$$

and if $1 \leq k \leq 2l$, then

$$\begin{aligned}
[L_3, L_+]u_k &= (L_3L_+ - L_+L_3)u_k \\
&= k(2l - (k-1))L_3u_{k-1} - (l-k)L_+u_k \\
&= k(2l - (k-1)(l - (k-1))u_{k-1} - (l-k)k(2l - (k-1))u_{k-1} \\
&= k(2l - (k-1))u_{k-1} = L_+u_k.
\end{aligned}$$

Therefore $[L_3, L_+] = L_3$ on V as desired. The other two commutation relations are similarly verified by direct calculation.

However we still must show that the representation defined via (18) is irreducible. Suppose that W is a nontrivial invariant subspace of V. We must show that $W = V$. Let $w \in W$ be nonzero, and decompose it as a linear combination of the basis vectors:

$$w = \sum_{k=0}^{2l} a_k u_k. \tag{19}$$

Because $w \neq 0$, at least one of the a_k's is nonzero. Let k_0 be the largest value of k for which $a_k \neq 0$ and consider

$$(L_+)^{k_0} w.$$

Since each application of L_+ decreases the index by 1, $(L_+)^{k_0}$ will eliminate every nonzero term in equation (19) except the $a_{k_0}u_{k_0}$ term, which after k_0 applications of L_+ becomes a nonzero multiple of u_0. Therefore $(L_+)^{k_0}w$ is a nonzero multiple of u_0, and since W is invariant, this means that u_0 belongs to W. But then $u_k = (L_-)^k u_0$ also belongs to W, so letting k range from 0 to $2l$ we find that every basis element is a member of W. Thus $W = V$ as desired. This completes the proof of Theorem 4.1. □

We started at the Lie algebra level because the calculations are more straightforward than at the Lie group level. Simply by finding a basis for V and showing that it satisfies the relations given in (18), we have classified all irreducible representations. But ultimately our goal is to return to Lie groups, because it is the representations of SO(3) that will correspond to solutions of the rotationally invariant Schrödinger equation.

Unfortunately this is not so easy. In our discussion of Lie algebras, we found that for every Lie group homomorphism Φ there is a corresponding Lie algebra homomorphism ϕ which relates to Φ as in equation (6). But we noted the converse—that every Lie algebra homomorphism has an associated Lie group homomorphism—is not true in general. In the next two subsections we investigate the consequences of this fact for the groups SU(2) and SO(3).

4.2 The Irreducible Representations of SU(2)

We begin with the associated irreducible representations of SU(2).

Theorem 4.4. *Let* $\pi_l : \mathrm{su}(2) \to \mathrm{gl}(V_l)$ *be an irreducible representation of* $\mathrm{so}(3)$ *with dimension* $\dim(V_l) = 2l + 1$*. Then there exists a representation* Π_l *of the Lie group* $\mathrm{SU}(2)$ *such that* $\Pi_l(e^X) = e^{\pi_l(X)}$ *for all* X *in* $\mathrm{su}(2)$*.*

This theorem is guaranteed to hold, since SU(2) is simply connected and every Lie algebra homomorphism has an associated Lie group homomorphism for simply connected Lie groups. However as we have already mentioned, this is a difficult statement to prove, so instead we rely on the explicit construction of the Π_l's given below.

A further point to note is that by Proposition 2.20, every irreducible representation of SU(2) corresponds to a unique irreducible representation of su(2). Therefore since the irreducible representations of su(2) are completely determined by the value l, the only irreducible representations of SU(2) are those described in the theorem.

Proof. We first construct a representation Π_l of SU(2) on the space of homogeneous polynomials of degree $2l$ in two complex variables, which we denote by V_l. By Theorem 2.16, there is an associated representation π_l of su(2), which is related to Π_l by the formula

$$\Pi_l(e^X) = e^{\pi_l(X)}, \tag{20}$$

for $X \in \mathrm{SU}(2)$. We will show that π_l is irreducible and hence is the unique $2l+1$ dimensional irreducible representation described in Theorem 4.1. Then by Proposition 2.20, Π_l is also irreducible, which completes the proof.

To begin, define for each $U \in \mathrm{SU}(2)$ a linear transformation $\Pi_l(U)$ on the space V_l by the formula

$$[\Pi_l(U)p](z) = p(U^{-1}z), \quad z \in \mathbb{C}^2. \tag{21}$$

We show that Π_l defined in this way is a representation of SU(2).

Elements of V_l have the form

$$p(z_1, z_2) = a_0 z_1^{2l} + a_1 z_1^{2l-1} z_2 + a_2 z_1^{2l-2} z_2^2 + \ldots + a_{2l} z_2^{2l} \tag{22}$$

with $z_1, z_2 \in \mathbb{C}$ and the a_j's arbitrary complex constants, from which we see that $\dim(V_l) = 2l + 1$. If p is as in equation (22), then writing out Π_l explicitly gives

$$[\Pi_l(U)p](z_1, z_2) = \sum_{k=0}^{2l} a_k (U_{11}^{-1} z_1 + U_{12}^{-1} z_2)^{2l-k} (U_{21}^{-1} z_1 + U_{22}^{-1} z_2)^k.$$

Expanding out the right hand-side of this formula shows that $\Pi_l(U)p$ is again a homogeneous polynomial of degree $2l$, so $\Pi_l(U)$ actually maps V_l into V_l. This verifies that Π_l is well-defined.

To see that Π_l is a representation, note that

$$\begin{aligned}\Pi_l(U_1)[\Pi_l(U_2)p](z) &= [\Pi_l(U_2)p](U_1^{-1}z) = p(U_2^{-1}U_1^{-1}z) \\ &= \Pi_l(U_1U_2)p(z).\end{aligned}$$

This calculation makes it clear that the inverse on the right-hand side of equation (21) is necessary for Π_l to be a representation, since it undoes the order reversal which occurs when applying $\Pi_l(U_1)$ and $\Pi_l(U_2)$.

Using Proposition 2.10 and equation (20), the associated representation π_l of su(2) can be computed as

$$\begin{aligned}(\pi_l(X)p)(z) &= \frac{d}{dt}(e^{t\pi_l(X)}p)(z)\bigg|_{t=0} = \frac{d}{dt}(\Pi_l(e^{tX})p)(z)\bigg|_{t=0} \\ &= \frac{d}{dt}p(e^{-tX}z)\bigg|_{t=0}.\end{aligned}$$

Now, let $z(t) = (z_1(t), z_2(t))$ be the curve in $\mathbb{C}^2$ defined as $z(t) = e^{-tX}z$. By the chain rule,

$$\pi_l(X)p = \frac{\partial p}{\partial z_1}\frac{dz_1}{dt}\bigg|_{t=0} + \frac{\partial p}{\partial z_2}\frac{dz_2}{dt}\bigg|_{t=0}.$$

But again by Proposition 2.10, $dz/dt|_{t=0} = -Xz$, so this equation becomes

$$\pi_l(X)p = -\frac{\partial p}{\partial z_1}(X_{11}z_1 + X_{12}z_2) - \frac{\partial p}{\partial z_2}(X_{21}z_1 + X_{22}z_2).$$

Applying this formula to the basis elements E_1, E_2, and E_3 of su(2) defined in the proof of Proposition 3.9, we find

$$\begin{aligned}\pi_l(E_1) &= \frac{i}{2}\left(-z_2\frac{\partial}{\partial z_1} - z_1\frac{\partial}{\partial z_2}\right) \\ \pi_l(E_2) &= \frac{1}{2}\left(z_2\frac{\partial}{\partial z_1} - z_1\frac{\partial}{\partial z_2}\right) \\ \pi_l(E_3) &= \frac{i}{2}\left(-z_1\frac{\partial}{\partial z_1} + z_2\frac{\partial}{\partial z_2}\right).\end{aligned}$$

We can now define L_+, L_-, and L_3 in a manner analogous to the operators used in the proof of Theorem 4.1. This gives operators

$$L_3 = \frac{1}{2}\left(z_1\frac{\partial}{\partial z_1} - z_2\frac{\partial}{\partial z_2}\right)$$
$$L_+ = -iz_1\frac{\partial}{\partial z_2}$$
$$L_- = -iz_2\frac{\partial}{\partial z_1}.$$

which act on a basis element $z_1^{2l-k}z_2^k$ for V_l in the following manner:

$$L_3(z_1^{2l-k}z_2^k) = (l-k)z_1^{2l-k}z_2^k$$
$$L_+(z_1^{2l-k}z_2^k) = -ikz_1^{2l-k+1}z_2^{k-1} \tag{23}$$
$$L_-(z_1^{2l-k}z_2^k) = -i(2l-k)z_1^{2l-k-1}z_2^{k+1}. \tag{24}$$

Therefore each $z_1^{2l-k}z_2^k$ is an eigenvector for L_3 while L_+ and L_- have the effect of shifting the exponent k of z_2 up or down by one. We can show that π_l is irreducible using the same argument as in the proof of Theorem 4.1, and hence it must be the unique $2l+1$ dimensional irreducible representation of su(2). By Proposition 2.20, Π_l is thus also irreducible and unique as desired. □

While interesting, the result we have just proved may not be particularly enlightening or surprising. The surprise comes in the next section, when we attempt to find the irreducible representations of SO(3). Whereas here a representation of SU(2) was found for every l, for SO(3) representations will only exist for *integer* values of l. The representations we constructed in this subsection will be essential to proving this fact.

4.3 The Irreducible Representations of SO(3)

The strange relationship between SU(2) and SO(3), which we saw with the 2-1 homomorphism, now comes into play. It is the irreducible representations of SO(3) that interest us in order to describe angular momentum, but because SO(3) is not simply connected we cannot find a representation for every value of l.

Theorem 4.5. *Let $\sigma_l : \mathrm{so}(3) \to \mathrm{gl}(V_l)$ be an irreducible representation of* so(3) *with dimension* $\dim V_l = 2l+1$ *(l is the spin of σ_l). If l is an integer (i.e., if the dimension of V is odd), then there exists a representation Σ_l of the Lie group* SO(3) *such that $\Sigma_l(e^X) = e^{\sigma_l(X)}$ for all X in* so(3)*. If l is a half-integer (i.e., if the dimension of V is even) then there is no such representation.*

Proof. Suppose first that l is a half-integer. Using Example 2.11, we find that

$$e^{2\pi F_3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(2\pi) & -\sin(2\pi) \\ 0 & \sin(2\pi) & \cos(2\pi) \end{pmatrix} = I.$$

On the other hand by Theorem 4.1 the operator $L_3 = i\sigma(F_3)$ defined in equation (15) is diagonal in the basis $\{u_j\}$, and its eigenvalues are half-integers. Therefore,

$$e^{2\pi\sigma_l(F_3)} = e^{2\pi i L_3} = -I.$$

Thus, if a corresponding representation Σ_l of SO(3) existed, we would have

$$I = \Sigma_l(I) = \Sigma_l(e^{2\pi F_3}) = e^{2\pi\sigma_l(F_3)} = -I,$$

which is a contradiction.

Suppose however that l is an integer. Because su(2) and so(3) are isomorphic, we can consider σ_l to be the composition of the Lie algebra representation ϕ associated to the 2-1 homomorphism and the representation π_l of su(2) defined in the proof of Theorem 4.4. In symbolic form, $\sigma_l = \pi_l \circ \phi^{-1}$.

The associated Lie group homomorphism would then be $\Sigma_l = \Pi_l \circ \Phi^{-1}$, where Π_l is the representation of SU(2) defined in Theorem 4.4 and Φ is the 2-1 homomorphism with kernel $\ker(\Phi) = \{I, -I\}$ discussed in Section 3. However this representation is not necessarily well-defined, since Φ is not an isomorphism and so 'Φ^{-1}' actually maps an element R of SO(3) to *two* elements of SU(2), U and $-U$.

$$\begin{array}{ccc} \mathrm{SU}(2) & \xrightarrow{\Pi_l} & \mathrm{GL}(V_l) \\ \downarrow \Phi & \nearrow \Sigma_l & \\ \mathrm{SO}(3) & & \end{array} \qquad \begin{array}{ccc} \mathrm{su}(2) & \xrightarrow{\pi_l} & \mathrm{gl}(V_l) \\ \downarrow \phi & \nearrow \sigma_l & \\ \mathrm{so}(3) & & \end{array}$$

When l is a half-integer, this problem leads to the contradiction we found above. But if l is an integer, then $\pi_l(E_3)$ is diagonal in the basis $\{z_1^{2l-k} z_2^k\}$ with integer eigenvalues, and therefore

$$\Pi_l(-I) = \Pi_l(e^{2\pi E_3}) = e^{\pi_l(2\pi E_3)} = I,$$

so in fact $\Pi_l(U) = \Pi_l(-U)$ for all $U \in \mathrm{SU}(2)$. Therefore it makes sense to define Σ_l as we have above, because in this case

$$\Sigma_l(R) = \Pi_l(\Phi^{-1}(R)) = \Pi_l(U) = \Pi_l(-U). \tag{25}$$

It is easy to show that Σ_l is a homomorphism and is continuous, so it is the desired representation of SO(3). □

This theorem should be deeply troubling. If the representations of SO(3) correspond to solutions to the rotationally invariant Schrödinger equation (on finite-dimensional subspaces of $L^2(\mathbb{R}^3)$), then it appears that half of the possible solutions are missing. The half-integer representations of so(3) could be dismissed as unphysical, but as we shall see in the next section, they are essential to describing the behavior of half-integer spin particles such as electrons. Fortunately a solution comes via 'projective' representations, which we will also discuss briefly in Section 5.

5 Solutions to the Schrödinger Equation

In this section we finally return to the problem of identifying solutions to the rotationally invariant Schrödinger equation. Equipped with a description of the irreducible representations of so(3) and SO(3), we can now determine the invariant subspaces of the angular momentum operators in $L^2(\mathbb{R}^3)$, from which we obtain the invariant subspaces of the Hamiltonian as stated in Proposition 1.2.

5.1 Realizing the Solutions in $L^2(\mathbb{R}^3)$

In subsection 4.1 we classified the irreducible representations of so(3) on an abstract vector space V. We saw that the angular momentum operators can be thought of as a representation of so(3) realized on a finite-dimensional invariant subspace of $L^2(\mathbb{R}^3)$. Thus we begin by attempting to identify, for each l, such an invariant subspace. We will find this subspace to be the space of spherical harmonics of degree l, multiplied by a radial function which depends on l and the potential V. However this subspace exists for only integer values of l, hinting back to the missing half-integer representations from the last section.

Theorem 5.1. *For each integer $l \geq 0$, the unique irreducible representation of* so(3) *may be realized as a $2l+1$ dimensional space V_l with a basis of eigenfunctions of the L_3 operator, which we call the space of **spherical harmonics** of degree l. These eigenfunctions are the angular part of solutions to the rotationally invariant Schrödinger equation.*

Proof. We start by returning to the angular momentum operators as defined in Section 1.2. Equation (3) gives each L_j as a differential operator, and writing these in spherical coordinates we have

$$L_1 = -i\hbar\left(-\sin(\phi)\frac{\partial}{\partial\theta} - \cos(\phi)\cot(\theta)\frac{\partial}{\partial\phi}\right)$$
$$L_2 = -i\hbar\left(+\cos(\phi)\frac{\partial}{\partial\theta} - \sin(\phi)\cot(\theta)\frac{\partial}{\partial\phi}\right)$$
$$L_3 = -i\hbar\frac{\partial}{\partial\phi}.$$

Note that these operators still obey the commutation relations from equation (4) and therefore still constitute a representation of so(3). Thus we can rely on the analysis in Section 4.1 in order to describe the space V_l. In particular, we are looking for eigenfunctions f_l^m of L_3, which for any given l will be a basis for V_l. These eigenfunctions are characterized by the values l and m as in equation (18) with $m = l - k$. Explicitly, we have

$$L^2 f_l^m = (L_1^2 + L_2^2 + L_3^2) f_l^m = \hbar^2 l(l+1) f_l^m;$$
$$L_3 f_l^m = \hbar m f_l^m \tag{26}$$

where $l = 0, 1/2, 1, 3/2, \ldots$ and $m = -l, -l+1, \ldots, l-1, l$. It is simple to check that the equation for L^2 holds by noting $L^2 = L_+L_- + L_3^2 - \hbar L_3$ and applying equation (18).

The eigenfunctions for a single l are connected in a chain by the L_+ and L_- operators (which is why their span is an irreducible representation of so(3). We will thus need to write L_+ and L_- as differential operators in spherical coordinates:

$$L_\pm = L_1 \pm iL_2 = -i\hbar\left[(-\sin\phi \pm i\cos\phi)\frac{\partial}{\partial\theta} - (\cos\phi \pm i\sin\phi)\cot\theta\frac{\partial}{\partial\phi}\right].$$

Using the identity $\cos\phi \pm i\sin\phi = e^{\pm i\phi}$, this gives

$$L_\pm = \pm\hbar e^{\pm i\phi}\left(\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}\right).$$

We are now able to determine $f_l^m(\theta,\phi)$ (which for now we simply call f) using the eigenvalue equations (26) and the partial derivative expressions for L_3, L_+, and L_-. First of all, f is an eigenfunction for L_3 with eigenvalue $\hbar m$:

$$L_3 f = -i\hbar\frac{\partial f}{\partial\phi} = \hbar m f,$$

so

$$f(\theta, \phi) = g(\theta)e^{im\phi}, \tag{27}$$

where g is a function on $\mathbb{R}^3$ that depends only on θ. Furthermore f is an eigenfunction of L^2 which we can express in terms of L_+, L_-, and L_3 to get

$$\begin{aligned} L^2 &= (L_+L_- + L_3^2 - \hbar L_3)f \\ &= \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)(-\hbar e^{-i\phi})\left(\frac{\partial f}{\partial\theta} - i\cot\theta\frac{\partial f}{\partial\phi}\right) - \hbar^2\frac{\partial^2 f}{\partial\phi^2} - \frac{\hbar^2}{i}\frac{\partial f}{\partial\phi} \\ &= \hbar^2 l(l+1)f. \end{aligned}$$

But from equation (27), we have $\partial f/\partial\theta = e^{im\phi}dg/d\theta$ and $\partial f/\partial\phi = ime^{im\phi}g$. Thus

$$\begin{aligned} -e^{i\phi}&\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)(e^{i(m-1)\phi}\left(\frac{dg}{d\theta} + mg\cot\theta\right) + m^2ge^{im\phi} - mge^{im\phi} \\ &= e^{im\phi}\Bigg[-\frac{d}{d\theta}\left(\frac{dg}{d\theta} + mg\cot\theta\right) + (m-1)\cot\theta\left(\frac{dg}{d\theta} + mg\cot\theta\right) \\ &\qquad +m(m-1)g\Bigg] = l(l+1)ge^{im\phi}. \end{aligned}$$

Canceling $e^{im\phi}$ and multiplying through by $-\sin^2\theta$, we obtain

$$\sin^2\theta\frac{d^2g}{d\theta^2} + \sin\theta\cos\theta\frac{dg}{d\theta} - m^2g = -l(l+1)\sin^2\theta g.$$

Or written more simply:

$$\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{dg}{d\theta}\right) + [l(l+1)\sin^2\theta - m^2]g = 0.$$

This is a differential equation for $g(\theta)$ with solution

$$g(\theta) = AP_l^m(\cos\theta),$$

where A is a constant and P_l^m is the **associated Legendre function** defined by

$$P_l^m(x) = (1-x^2)^{|m|/2}\left(\frac{d}{dx}\right)^{|m|}P_l(x).$$

Here $P_l(x)$ is the lth Legendre polynomial, which we can define by the **Rodrigues formula**:

$$P_l(x) = \frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l(x^2-1)^l.$$

Eigenfunctions for the angular momentum operators will therefore take the form

$$f_l^m(\theta, \phi) = Ae^{im\phi} P_l^m(\cos\theta) \tag{28}$$

for a constant A (which in general could depend on r). When normalized, this function is called a **spherical harmonic** and denoted Y_l^m. The spherical harmonics may seem complicated, but for our purposes it is enough to know that they exist and that the $2l+1$ functions for any given l constitute an irreducible representation of so(3).

But for what values of l and m does Y_l^m exist? First of all, note that for in order for Y_l^m to be single-valued, we must have

$$e^{im\phi} = e^{im(\phi+2\pi)},$$

from which we see that m must be an integer. This requirement can be seen directly in the equation for the Legendre function, where m must be an integer in order for the mth derivative to make sense. Similarly from the Rodrigues formula we see that l must be a non-negative integer. In other words, we obtain the integer representations of so(3) but not the half-integer representations.

Finally, note that because the spherical harmonics are eigenfunctions of the angular momentum operators, they are also eigenfunctions of the Hamiltonian and therefore constitute solutions to the rotationally invariant Schrödinger equation. □

The above analysis gives the angular dependence of the Schrödinger equation as a representation of so(3), but in order to obtain a full solution we must describe the radial dependence as well. Because we are dealing with rotationally invariant systems, we can separate the radial and angular parts of the wavefunction as described below, which gives a differential equation in terms of r that we can then solve.

Theorem 5.2. *Eigenfunctions of the Hamiltonian for the rotationally invariant Schrödinger equation take the form*

$$\psi(\theta, \phi, r) = Y(\theta, \phi)R(r) = Y(\theta, \phi)\frac{u(r)}{r}$$

where Y is a spherical harmonic of degree l and R is a radial function which depends on l. If we apply the Schrödinger equation to ψ, the angular and radial parts of the equation factor apart and we find that $u(r) = rR(r)$ satisfies the differential equation

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu \tag{29}$$

We will not go so far as to solve this differential equation for $u(r)$, since we would need a specific potential V in order to do so.

Proof. The first part of the theorem we have already shown above by proving the angular function is of the form in equation (28). To show that $u(r)$ satisfies equation (29), we need only show that

$$\nabla^2\psi(\theta,\phi,r) = \frac{1}{r}Y(\theta,\phi)\left[\frac{d^2u}{dr^2} - \frac{l(l+1)}{r^2}u(r)\right] \tag{30}$$

which gives the desired equation when plugged into the TISE.

We will make use of the following identity, which is easy to prove by expressing the L^2 operator in angular coordinates:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{L^2}{\hbar^2 r^2} \tag{31}$$

To begin, consider the case $l = 0$, in which case Y_l^m is just a constant which we take to be 1. Then in cartesian coordinates

$$\begin{aligned}\frac{\partial}{\partial x_j}R(r) &= \frac{dR}{dr}\frac{d}{dx_j}\sqrt{x_1^2+x_2^2+x_3^2}\\ &= \frac{dR}{dr}\frac{x_j}{r}\end{aligned}$$

and so

$$\begin{aligned}\sum_{j=1}^{3}\frac{\partial^2}{\partial x_j^2}R(r) &= \sum_{j=1}^{3}\left[\frac{d^2R}{dr^2}\frac{x_j^2}{r^2} + \frac{df}{dr}\left(\frac{1}{r} - \frac{x_j^2}{r^3}\right)\right]\\ &= \frac{d^2R}{dr^2} + \frac{2}{r}\frac{df}{dr} = \frac{1}{r}\frac{d^2u}{dr^2}.\end{aligned}$$

For the general case, the product rule for the Laplacian gives us

$$\nabla^2\psi = (\nabla^2 Y)R(r) + 2\nabla Y\cdot\nabla R(r) + Y\nabla^2 R(r). \tag{32}$$

There are three points to note. First, using equation (31) and the fact that Y is an eigenfunction for L^2 with eigenvalue $\hbar^2 l(l+1)$, we may rewrite the Laplacian of Y as

$$\nabla^2 Y = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)Y - \frac{L^2}{\hbar r^2}Y = -\frac{l(l+1)}{r^2}Y$$

where the radial term drops out because Y has no r dependence. Second, we can again use equation (31) to rewrite the Laplacian of $R(r)$ as

$$\nabla^2 R(r) = \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) R(r)$$

where this time the L^2 term drops out. Third, the cross term $2\nabla Y \cdot \nabla R(r)$ is zero, because it is the dot product of a purely angular and a purely radial vector.

Substituting these changes into equation (32) and simplifying results in the equation

$$\nabla^2 \psi(\theta, \phi, r) = Y(\theta, \phi) \left[\frac{d^2 R}{dr^2} + \frac{2}{r}\frac{dR}{dr} - \frac{l(l+1)}{r^2} R(r)\right].$$

From here it is a simple matter of changing variables from R to u to obtain the desired expression (30). □

To give a summary of this section, we began by finding the eigenfunctions of the angular momentum operators and showing that these are the solutions to the angular part of the rotationally invariant Schrödinger equation. Now because $\hat{H}$ and L_j commute, these are also the solutions of $\hat{H}$ so in fact we have found the eigenfunctions of $\hat{H}$ and thus completely classified all solutions to the TISE with rotational symmetry.

However, we did not obtain every possible value of l. The half-integer values, which appeared as representations of so(3) in Section 4, do not appear as solutions to the TISE. To explain this, we must return to the result from Section 4.3. As we have already mentioned, the angular momentum operators constitute an action of so(3) which is associated to the natural action of SO(3)

$$(\Pi(R)\psi)(\mathbf{x}) = \psi(R^{-1}\mathbf{x}).$$

Any invariant subspace of L_1, L_2, and L_3 will, by Proposition 2.20, also be invariant under this action and thus constitute a representation of SO(3). From this perspective, it is obvious that the half-integer representations (i.e., the even dimensional invariant subspaces) since these would produce half-integer representations of SO(3) which we have shown cannot exist.

It may seem that we are laboring over a trivial point. There are no even dimensional invariant subspaces of the rotationally invariant Schrödinger equation, and why not leave it at that? But the situation is not that simple. In the next section we will discuss the quantum mechanical property of spin (or intrinsic angular momentum), which for fermionic particles such as electrons requires an explanation via the half-integer representations. Thus we must find some way to reintroduce them, which we will do by changing the function space and defining projective representations.

5.2 Spin and Projective Representations

So far we have been working with wavefunctions in the space $L^2(\mathbb{R}^3) = L^2(\mathbb{R}^3, \mathbb{C})$, but various experiments in physics (most notably the Stern-Gerlach experiment) have shown that this space requires a modification to include what has been dubbed the 'spin' of a particle, which can be thought of as intrinsic angular momentum. Spin comes in half-integer multiples of $\hbar$ and acts analogously to orbital angular momentum. From a mathematical perspective, it is just a finite-dimensional representation of so(3) like that discussed in Section 4 (hence giving the value l the title spin in the proof of Theorem 4.1).

In order to account for spin, we modify the function space by taking a tensor product with a finite-dimensional vector space V_l that carries an action of so(3) and has spin l. Thus the new solution space is $L^2(\mathbb{R}^3) \otimes V_l$, and we hope to find an action of the group SO(3) on this space. This is all well and good when l is an integer, as the actions on $L^2(\mathbb{R}^3)$ and V_l will carry over to the tensor product. But for half-integer spin particles (commonly known as fermions), the space V_l will not carry an ordinary action of SO(3), so $L^2(\mathbb{R}^3) \otimes V_l$ will not either. In order to solve this problem, we introduce projective representations:

Definition 5.3. Let $G \in M_n(\mathbb{C})$ be a matrix Lie group and V be a finite-dimensional vector space over $\mathbb{C}$. A finite-dimensional **projective representation** of G is a Lie group homomorphism Π of G into the quotient group $\mathrm{GL}(V)/\{e^{i\theta} I\}$, where $\{e^{i\theta} I\}$ denotes the group of matrices of the form $e^{i\theta}$, $\theta \in \mathbb{R}$.

A projective representation is exactly the same as an ordinary Lie group representation, except that the operators on the space V are now equivalence classes of operators. Two operators are equivalent if they differ only by a complex constant with magnitude 1, so in particular I and $-I$ become the same operator, and so do U and $-U$.

If we consider not ordinary, but *projective* representations of SO(3) on $L^2(\mathbb{R}^3) \otimes V_l$, we find that the half-integer representations do appear. Looking back to Section 4.3, we see that the contradiction derived in the proof of Theorem 4.5 is no longer a concern, because in the projective representation I and $-I$ are equivalent. Thus we are free to define $\Sigma_l(R)$ as in equation (25), and Σ_l defined in this way will be the projective representation associated to σ_l.

Projective representations of SO(3) on the space $L^2(\mathbb{R}^3) \otimes V_l$ are the conclusion of our analysis, since by describing them we describe all eigenfunctions, and thus all possible solutions, to the rotationally invariant Schrödinger equation for both integer and half-integer spin. We conclude this section by considering the all important case of $l = 1/2$, which describes the angular momentum of electrons and plays an important role in describing the hydrogen atom.

Example 5.4. The function space for the case $l = 1/2$ is $L^2(\mathbb{R}^3) \otimes V_l$ where V_l is a two-dimensional vector space carrying an action of the Lie algebra so(3). It turns out this function space is isomorphic to $L^2(\mathbb{R}^3, \mathbb{C}^2)$, so we can define a projective action Π of the group SO(3)

$$(\Pi(R)\psi)(\mathbf{x}) = U\psi(R^{-1}\mathbf{x}) \tag{33}$$

where R is an element of SO(3) and U one of the two elements of SU(2) associated to R by the 2-1 homomorphism Φ (the other being $-U$). We can think of R as rotating the orbital wavefunction, while U rotates the spin vector which is the 2-d complex 'orientation' of the wavefunction.

Recall the standard representations of SO(3) on $L^2(\mathbb{R}^3)$ described in Section 4. Changing the codomain from $\mathbb{C}$ to $\mathbb{C}^2$ (or equivalently taking the tensor with a two-dimensional vector space) doubles the dimension of these representations, so that we now obtain not the integer, but the half-integer representations.

There are two last points to note. First, the representation of so(3) on V_l is simply the standard representation, which in this case is the identity. Thus the basis vectors E_1, E_2, and E_3 get mapped to themselves, which explains the origin of the Pauli spin matrices for spin-1/2 particles. Second, applying equation (33) to the identity gives two interpretations:

$$(\Pi(I)\psi)(\mathbf{x}) = \psi(\mathbf{x}) \quad \text{and} \quad (\Pi(I)\psi)(\mathbf{x}) = -\psi(\mathbf{x}).$$

The first equation corresponds to the trivial rotation, while the second corresponds to a rotation by 360°. The reason we obtain two answers is that there are two non-equivalent paths to the identity through SO(3), which is because SO(3) is not simply connected and has fundamental group $\mathbb{Z}_2$. This explains the oft-heard statement that applying a 360° rotation to an electron returns the negative of the original wavefunction. Of course, in the projective representation the two are equivalent.

6 Conclusion

The purpose of this paper has been to give a clear explanation of the mathematics behind quantum mechanical angular momentum, and how it can be applied to find solutions to the rotationally invariant Schrödinger equation. We gave an overview of Lie theory and introduce the groups SU(2) and SO(3). The irreducible representations of these groups and their Lie algebras describe the invariant subspaces of the angular momentum operators and the rotationally invariant Schrödinger equation. Importantly, not all representations appear directly, but instead must be found using projective representations. This is because the group SO(3) is not simply connected, which results in the unusual behavior of spin-1/2 particles where a 360° rotation results in the minus of the wavefunction.

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