Angular Momentum To 3D Hydrogen Atom

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1 Rotations as a Physical Symmetry

A *spatial rotation* is a linear map on $\mathbb{R}^3$ that preserves lengths and orientation. Equivalently, a rotation is a real 3×3 matrix R such that

$$R^\top R = I, \tag{1.1}$$

$$\det R = 1. \tag{1.2}$$

The set of all such matrices is denoted

$$SO(3) \;=\; \{\, R \in \mathbb{R}^{3\times 3} \mid R^\top R = I,\ \det R = 1 \,\}. \tag{1.3}$$

It is closed under matrix multiplication and inverses, hence it is a group under multiplication.

1.1 Infinitesimal Rotations and $\mathfrak{so}(3)$

Physics uses *continuous* rotations (we can rotate by arbitrarily small angles). So we consider a smooth one-parameter family of rotations

$$R(\varepsilon) \in SO(3), \qquad R(0) = I, \tag{1.4}$$

and expand for small ε:

$$R(\varepsilon) = I + \varepsilon A + O(\varepsilon^2), \tag{1.5}$$

for some real matrix A (the "infinitesimal generator" at the identity).

Theorem 1.1. *A is antisymmetric.*

$$A^\top = -A$$

Proof. Insert (1.5) into orthogonality (1.1):

$$\begin{aligned} I = R(\varepsilon)^\top R(\varepsilon) &= (I + \varepsilon A)^\top (I + \varepsilon A) + O(\varepsilon^2) \\ &= (I + \varepsilon A^\top)(I + \varepsilon A) + O(\varepsilon^2) \\ &= I + \varepsilon (A^\top + A) + O(\varepsilon^2). \end{aligned} \tag{1.6}$$

Equating the $O(\varepsilon)$ term to zero gives

$$A^\top + A = 0 \quad \Longleftrightarrow \quad A^\top = -A, \tag{1.7}$$

□

Any infinitesimal rotation can be represented by an antisymmetric matrices. Thus the space of all possible infinitesimal generators at the identity is

$$\mathfrak{so}(3) := \{\, A \in \mathbb{R}^{3\times 3} \mid A^\top = -A \,\}. \tag{1.8}$$

1.2 Geometric Representation of Infinitesimal Rotations

Let ε_{ijk} be the Levi-Civita symbol ($\varepsilon_{123} = +1$, fully antisymmetric). Define three matrices $\{L_x, L_y, L_z\}$ (also written L_1, L_2, L_3) by components

$$(L_i)_{jk} = -\,\varepsilon_{ijk}. \tag{1.9}$$

Explicitly,

$$L_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad L_y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad L_z = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{1.10}$$

Any antisymmetric $A \in \mathfrak{so}(3)$ can be written as a linear combination

$$A(\boldsymbol{\omega}) = \sum_{i=1}^{3} \omega_i L_i, \tag{1.11}$$

for some real vector $\boldsymbol{\omega} = (\omega_1, \omega_2, \omega_3)$.

Theorem 1.2. *Let $\boldsymbol{\omega} \in \mathbb{R}^3$ be a vector and $A(\boldsymbol{\omega}) \in \mathfrak{so}(3)$ be the corresponding Lie algebra element defined by $A(\boldsymbol{\omega}) = \sum_i \omega_i L_i$. For any $v \in \mathbb{R}^3$,*

$$A(\boldsymbol{\omega})v = \boldsymbol{\omega} \times v. \tag{1.12}$$

Proof. We compute the action componentwise. For $v \in \mathbb{R}^3$, the j-th component is:

$$\begin{aligned}
\big(A(\boldsymbol{\omega})v\big)_j &= \sum_k \big(A(\boldsymbol{\omega})\big)_{jk} v_k \\
&= \sum_k \left(\sum_i \omega_i (L_i)_{jk} \right) v_k \\
&= \sum_{i,k} \omega_i (-\varepsilon_{ijk}) v_k \\
&= \sum_{i,k} \varepsilon_{jik}\, \omega_i v_k = (\boldsymbol{\omega} \times v)_j.
\end{aligned} \tag{1.13}$$

Since this holds for all components j, the equality is proven. This confirms that the infinitesimal rotation generated by $A(\boldsymbol{\omega})$ acts as a cross product with the axis-angle vector $\boldsymbol{\omega}$. □

1.3 Noncommutativity of Infinitesimal Rotations

Fix axes i and j and define a small rotation about axis i by

$$R_i(\varepsilon) := I + \varepsilon L_i + O(\varepsilon^2). \tag{1.14}$$

To measure the failure of commutativity, form the *group commutator*

$$C_{ij}(\varepsilon) := R_i(\varepsilon)\, R_j(\varepsilon)\, R_i(\varepsilon)^{-1}\, R_j(\varepsilon)^{-1}. \tag{1.15}$$

If rotations commuted, then $C_{ij}(\varepsilon) = I$. The leading deviation from I is the geometric "leftover rotation".

Theorem 1.3. *The generators $\{L_i\}$ of $\mathfrak{so}(3)$ satisfy the commutation relations*

$$[L_i, L_j] = \sum_{k=1}^{3} \varepsilon_{ijk} L_k. \tag{1.16}$$

Physically, this matrix commutator governs the non-commutativity of infinitesimal rotations, appearing as the leading order term in the group commutator expansion:

$$R_i(\varepsilon) R_j(\varepsilon) R_i(\varepsilon)^{-1} R_j(\varepsilon)^{-1} = I + \varepsilon^2 [L_i, L_j] + O(\varepsilon^3). \tag{1.17}$$

Proof. First, to motivate the relevance of the commutator, we expand the rotation matrices $R_i(\varepsilon) = I - \varepsilon L_i + O(\varepsilon^2)$ and $R_i(\varepsilon)^{-1} = I + \varepsilon L_i + O(\varepsilon^2)$. Multiplying the terms up to order ε^2:

$$\begin{aligned}
C_{ij}(\varepsilon) &= (I - \varepsilon L_i)(I - \varepsilon L_j)(I + \varepsilon L_i)(I + \varepsilon L_j) + O(\varepsilon^3) \\
&= I + \varepsilon^2 (L_i L_j - L_j L_i) + O(\varepsilon^3)
\end{aligned}$$

$$= I + \varepsilon^2 [L_i, L_j] + O(\varepsilon^3). \tag{1.18}$$

We now calculate $[L_i, L_j]$ explicitly using the component definition $(L_i)_{ab} = -\varepsilon_{iab}$. The product is:

$$(L_i L_j)_{ab} = \sum_k (L_i)_{ak}(L_j)_{kb} = \sum_k \varepsilon_{iak}\varepsilon_{jkb}. \tag{1.19}$$

Using the Levi-Civita contraction identity $\sum_k \varepsilon_{iak}\varepsilon_{jkb} = \delta_{ij}\delta_{ab} - \delta_{ib}\delta_{aj}$, we find:

$$(L_i L_j)_{ab} = \delta_{ij}\delta_{ab} - \delta_{ib}\delta_{aj}, \quad (L_j L_i)_{ab} = \delta_{ij}\delta_{ab} - \delta_{jb}\delta_{ai}. \tag{1.20}$$

Subtracting these yields the commutator components:

$$\begin{aligned} ([L_i, L_j])_{ab} &= \delta_{jb}\delta_{ai} - \delta_{ib}\delta_{aj} \\ &= -\big(\delta_{ai}\delta_{bj} - \delta_{aj}\delta_{bi}\big) \\ &= -\sum_k \varepsilon_{ijk}\varepsilon_{kab} = \sum_k \varepsilon_{ijk}(L_k)_{ab}. \end{aligned} \tag{1.21}$$

Thus, $[L_i, L_j] = \sum_k \varepsilon_{ijk} L_k$. □

Combine (1.18) and (1.16):

$$C_{ij}(\varepsilon) = I + \varepsilon^2 \varepsilon_{ijk} L_k + O(\varepsilon^3). \tag{1.22}$$

Since $I + \theta L_k + O(\theta^2)$ is a rotation by small angle θ about axis k, (1.22) says: *do a small rotation about* i*, then about* j*, then undo both: the net effect is another small rotation of order* ε^2 *about the* k*-axis, with orientation set by* ε_{ijk}.

1.4 Unitary Representation $U(R)$ and Generators J

A rotation is a symmetry: it must preserve all probabilities. If $|\psi\rangle$ is a state and $U(R)$ implements rotation R, then inner products must be preserved:

$$\langle\psi|\psi\rangle = \langle U(R)\psi|U(R)\psi\rangle = \langle\psi|U(R)^\dagger U(R)|\psi\rangle \quad \forall|\psi\rangle. \tag{1.23}$$

Hence

$$U(R)^\dagger U(R) = I, \tag{1.24}$$

so $U(R)$ is unitary. Consistency of doing rotations in sequence requires the representation property

$$U(R_1 R_2) = U(R_1)U(R_2), \qquad U(I) = I. \tag{1.25}$$

Theorem 1.4. *Let* $U_i(\varepsilon)$ *be a unitary operator representing an infinitesimal rotation about axis* i*. If we define the generator* J_i *by the expansion*

$$U_i(\varepsilon) = I - \frac{i}{\hbar}\varepsilon J_i + O(\varepsilon^2), \tag{1.26}$$

then J_i *must be a Hermitian operator (*$J_i^\dagger = J_i$*).*

Proof. We begin with a general infinitesimal expansion $U_i(\varepsilon) = I + \varepsilon K_i + O(\varepsilon^2)$. The unitarity condition $U^\dagger U = I$ implies:

$$\begin{aligned} I = U_i(\varepsilon)^\dagger U_i(\varepsilon) &= (I + \varepsilon K_i)^\dagger (I + \varepsilon K_i) + O(\varepsilon^2) \\ &= I + \varepsilon(K_i^\dagger + K_i) + O(\varepsilon^2). \end{aligned} \tag{1.27}$$

Comparing terms of order ε, we require $K_i^\dagger + K_i = 0$, or $K_i^\dagger = -K_i$. Thus, the generator K_i is anti-Hermitian.

To correspond with physical observables, we adopt the convention $K_i = -iJ_i/\hbar$. Substituting this into the anti-Hermiticity condition:

$$\left(-\frac{i}{\hbar}J_i\right)^\dagger = -\left(-\frac{i}{\hbar}J_i\right) \implies \frac{i}{\hbar}J_i^\dagger = \frac{i}{\hbar}J_i \implies J_i^\dagger = J_i. \tag{1.28}$$

This confirms that J_i is Hermitian. (For finite rotations, this integrates to the exponential form $U(\hat{\boldsymbol{n}}, \phi) = \exp\left[-\frac{i}{\hbar}\phi(\hat{\boldsymbol{n}} \cdot \mathbf{J})\right]$). □

1.5 The Angular Momentum Commutators $[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k$

We now *import the geometric noncommutativity* encoded in $C_{ij}(\varepsilon)$ into Hilbert space. Consider the corresponding operator product

$$U(C_{ij}(\varepsilon)) = U_i(\varepsilon)\, U_j(\varepsilon)\, U_i(\varepsilon)^{-1}\, U_j(\varepsilon)^{-1}. \tag{1.29}$$

Using (1.26) and $U_i(\varepsilon)^{-1} = U_i(-\varepsilon)$, expand to $O(\varepsilon^2)$:

$$\begin{aligned} U(C_{ij}(\varepsilon)) &= \left(I - \frac{i}{\hbar}\varepsilon J_i\right)\left(I - \frac{i}{\hbar}\varepsilon J_j\right)\left(I + \frac{i}{\hbar}\varepsilon J_i\right)\left(I + \frac{i}{\hbar}\varepsilon J_j\right) + O(\varepsilon^3) \\ &= I - \frac{\varepsilon^2}{\hbar^2}[J_i, J_j] + O(\varepsilon^3). \end{aligned} \tag{1.30}$$

On the *spatial* side, we already derived (1.22): $C_{ij}(\varepsilon)$ is a rotation of size ε^2 about axis k with coefficient ε_{ijk}. Therefore, its quantum implementation must match an infinitesimal rotation about k:

$$U(C_{ij}(\varepsilon)) = U_k(\varepsilon^2\varepsilon_{ijk}) = I - \frac{i}{\hbar}(\varepsilon^2\varepsilon_{ijk})J_k + O(\varepsilon^3). \tag{1.31}$$

Equate the $O(\varepsilon^2)$ terms in (1.30) and (1.31):

$$-\frac{1}{\hbar^2}[J_i, J_j] = -\frac{i}{\hbar}\varepsilon_{ijk}J_k \quad \implies \quad [J_i, J_j] = i\hbar\,\varepsilon_{ijk}J_k. \tag{1.32}$$

2 Angular-Momentum Algebra

From Section 1 we obtained three Hermitian generators J_x, J_y, J_z implementing rotations, and we now want to classify the possible quantum states *purely from their algebra*, before choosing any coordinate representation.

Postulate (Rotation algebra). We assume the generators satisfy the commutation relations

$$[J_i, J_j] = i\hbar\, \varepsilon_{ijk} J_k, \qquad i, j, k \in \{x, y, z\}, \tag{2.1}$$

and are Hermitian:

$$J_i^\dagger = J_i. \tag{2.2}$$

Measurements correspond to Hermitian operators. A *Complete Set of Commuting Observables (CSCO)* is a collection of mutually commuting Hermitian operators whose joint eigenvalues label states uniquely (up to phase). In rotational problems, the natural commuting set will include:

- a rotational invariant (the analogue of "total angular momentum magnitude");
- one chosen component (the analogue of "projection onto a fixed axis").

Theorem 2.1. *If two Hermitian operators $\hat{A}$ and $\hat{B}$ commute ($[\hat{A}, \hat{B}] = 0$) and $\hat{A}$ is **non-degenerate**, then each eigenvector of $\hat{A}$ is also an eigenvector of $\hat{B}$. Consequently, there exists a unique common orthonormal basis.*

Proof. Let $|\phi_n\rangle$ be an eigenvector of $\hat{A}$ with eigenvalue a_n:

$$\hat{A}\,|\phi_n\rangle = a_n\,|\phi_n\rangle \tag{2.3}$$

Consider the action of $\hat{A}$ on the vector $\hat{B}\,|\phi_n\rangle$. Using the commutation property $\hat{A}\hat{B} = \hat{B}\hat{A}$:

$$\hat{A}(\hat{B}\,|\phi_n\rangle) = \hat{B}(\hat{A}\,|\phi_n\rangle) = \hat{B}(a_n\,|\phi_n\rangle) = a_n(\hat{B}\,|\phi_n\rangle) \tag{2.4}$$

This implies that the vector $(\hat{B}\,|\phi_n\rangle)$ is an eigenvector of $\hat{A}$ with eigenvalue a_n.

Since $\hat{A}$ is **non-degenerate**, the eigenspace corresponding to a_n is 1-dimensional. Therefore, the vector $\hat{B}\,|\phi_n\rangle$ must be proportional to $|\phi_n\rangle$ (linear dependence):

$$\hat{B}\,|\phi_n\rangle = b_n\,|\phi_n\rangle \tag{2.5}$$

where b_n is a scalar. Thus, $|\phi_n\rangle$ is simultaneously an eigenvector of $\hat{B}$. □

Remark 2.2. If $\hat{A}$ possesses **degenerate** eigenvalues, $\hat{B}\,|\phi_n\rangle$ is still an eigenvector of $\hat{A}$, but it is not necessarily proportional to $|\phi_n\rangle$. In this case, a common basis still exists, but it is not unique; there are infinite possible orthonormal basis sets common to both operators.

2.1 The Casimir J^2

We now identify the canonical rotational invariant: a scalar built from (J_x, J_y, J_z) that commutes with *all* components. This operator will label irreducible "multiplets" of rotation.

Definition 2.3 (Total angular momentum operator)**.** Define

$$J^2 \;:=\; J_x^2 + J_y^2 + J_z^2. \tag{2.6}$$

Theorem 2.4 (J^2 commutes with all generators)**.** *For each $i \in \{x, y, z\}$,*

$$[J^2, J_i] = 0. \tag{2.7}$$

Proof. Use the identity $[AB, C] = A[B, C] + [A, C]B$:

$$[J^2, J_i] = \sum_{k\in\{x,y,z\}} [J_k^2, J_i]$$
$$= \sum_k \Big(J_k[J_k, J_i] + [J_k, J_i]J_k \Big). \tag{2.8}$$

By (2.1), $[J_k, J_i] = i\hbar\, \varepsilon_{ki\ell} J_\ell$, hence

$$[J^2, J_i] = i\hbar \sum_{k,\ell} \varepsilon_{ki\ell} \big(J_k J_\ell + J_\ell J_k \big) = i\hbar \sum_{k,\ell} \varepsilon_{ki\ell} \{J_k, J_\ell\}, \tag{2.9}$$

where $\{A, B\} = AB + BA$ is the anticommutator. The tensor $\varepsilon_{ki\ell}$ is antisymmetric in (k, ℓ), while $\{J_k, J_\ell\}$ is symmetric in (k, ℓ), so the sum vanishes:

$$\sum_{k,\ell} \varepsilon_{ki\ell} \{J_k, J_\ell\} = 0.$$

Therefore $[J^2, J_i] = 0$. □

Corollary 2.5 (Simultaneous eigenkets of J^2 and J_z)**.** *Since $[J^2, J_z] = 0$, by Theorem 2.1, there exists a common orthonormal basis for the operators J^2 and J_z. We label these simultaneous eigenkets by their respective eigenvalues λ and $\hbar m$:*

$$J^2|\lambda, m\rangle = \lambda\, |\lambda, m\rangle, \qquad J_z|\lambda, m\rangle = \hbar m\, |\lambda, m\rangle. \tag{2.10}$$

2.2 Ladder Operators $J_\pm$

The operator J_z measures "projection" on a chosen axis. We now build operators that change the J_z eigenvalue in controlled steps, allowing us to generate the full spectrum algebraically.

Definition 2.6 (Ladder operators)**.** Justified by Appendix A, we define

$$J_\pm \;:=\; J_x \pm i J_y. \tag{2.11}$$

Theorem 2.7 (Adjoint relation)**.**

$$(J_+)^\dagger = J_-. \tag{2.12}$$

Proof. By (2.2), $J_x^\dagger = J_x$ and $J_y^\dagger = J_y$, hence

$$(J_x + iJ_y)^\dagger = J_x - iJ_y.$$

□

Theorem 2.8 ($J_\pm$ shifts the J_z eigenvalue)**.** *The commutators are*

$$[J_z, J_\pm] = \pm\hbar\, J_\pm. \tag{2.13}$$

Proof. From (2.1),

$$[J_z, J_x] = i\hbar J_y, \qquad [J_z, J_y] = -i\hbar J_x.$$

Therefore

$$[J_z, J_\pm] = [J_z, J_x] \pm i[J_z, J_y] = i\hbar J_y \pm i(-i\hbar J_x) = \pm\hbar(J_x \pm iJ_y) = \pm\hbar J_\pm.$$

□

Corollary 2.9 (Step action on eigenkets). *If* $J_z|\lambda, m\rangle = \hbar m|\lambda, m\rangle$, *then*

$$J_z\big(J_\pm|\lambda, m\rangle\big) = \hbar(m \pm 1)\big(J_\pm|\lambda, m\rangle\big). \tag{2.14}$$

Proof. Compute using (2.13):

$$J_z(J_\pm|\lambda, m\rangle) = (J_\pm J_z + [J_z, J_\pm])|\lambda, m\rangle = \hbar(m \pm 1)(J_\pm|\lambda, m\rangle).$$

□

Theorem 2.10 (Commutators with J^2).

$$[J^2, J_\pm] = 0. \tag{2.15}$$

Proof. Since $[J^2, J_i] = 0$ for each component J_i by Theorem 2.4,

$$[J^2, J_\pm] = [J^2, J_x] \pm i[J^2, J_y] = 0.$$

□

Theorem 2.11 (Useful identities for $J_\mp J_\pm$).

$$J_+J_- = J^2 - J_z^2 + \hbar J_z, \tag{2.16}$$
$$J_-J_+ = J^2 - J_z^2 - \hbar J_z. \tag{2.17}$$

Proof. Expand using (2.11):

$$\begin{aligned} J_+J_- &= (J_x + iJ_y)(J_x - iJ_y) = J_x^2 + J_y^2 + i(J_yJ_x - J_xJ_y) \\ &= J_x^2 + J_y^2 + i[J_y, J_x] = J_x^2 + J_y^2 + \hbar J_z, \end{aligned}$$

since $[J_x, J_y] = i\hbar J_z \Rightarrow [J_y, J_x] = -i\hbar J_z$. Using $J_x^2 + J_y^2 = J^2 - J_z^2$ gives (2.16). The proof of (2.17) is analogous. □

2.3 Eigenvalue Spectrum: j, m Bounds and Quantization

We now use only: (i) the commutators, (ii) Hermiticity, and (iii) positivity of norms to show the spectrum must be discrete and labeled by two quantum numbers j and m.

Lemma 2.12 (Positivity constraints). *For any state* $|\psi\rangle$,

$$\|J_\pm|\psi\rangle\|^2 = \langle\psi|J_\mp J_\pm|\psi\rangle \geqslant 0. \tag{2.18}$$

Proof. $\|J_\pm|\psi\rangle\|^2 = \langle\psi|J_\pm^\dagger J_\pm|\psi\rangle$ and $J_\pm^\dagger = J_\mp$ by Theorem 2.7. □

Theorem 2.13 (Discrete ladder in m and existence of top/bottom). *Let* $|\lambda, m\rangle$ *satisfy* (2.10). *Then:*

1. *Repeated application of* J_+ *produces eigenkets with* $m \mapsto m + 1$ *(unless it becomes zero), and similarly* J_- *produces* $m \mapsto m - 1$.
2. *There exist* $m_{\max}$ *and* $m_{\min}$ *such that*

$$J_+|\lambda, m_{\max}\rangle = 0, \qquad J_-|\lambda, m_{\min}\rangle = 0. \tag{2.19}$$

Proof. Part (1) is Corollary 2.9. For part (2), suppose there were no top state. Then m could be raised indefinitely while λ remains fixed (since $[J^2, J_+] = 0$). But using Lemma 2.12 and identity (2.17),

$$\begin{aligned} \|J_+|\lambda, m\rangle\|^2 &= \langle\lambda, m|J_-J_+|\lambda, m\rangle \\ &= \langle\lambda, m|(J^2 - J_z^2 - \hbar J_z)|\lambda, m\rangle \\ &= \lambda - \hbar^2 m^2 - \hbar^2 m = \lambda - \hbar^2 m(m+1) \geqslant 0. \end{aligned} \tag{2.20}$$

For sufficiently large m, the term $\hbar^2 m(m+1)$ exceeds λ, contradicting (2.20). Hence a maximal $m_{\max}$ exists with $J_+|\lambda, m_{\max}\rangle = 0$. The argument for $m_{\min}$ using J_- and (2.16) is identical. □

Theorem 2.14 (Form of the J^2 eigenvalue and allowed m values)**.** *Let* $m_{\max}$ *be as in* (2.19)*. Define*

$$j := m_{\max}. \tag{2.21}$$

Then

$$\lambda = \hbar^2 j(j+1), \tag{2.22}$$
$$m \in \{-j, -j+1, \dots, j-1, j\}. \tag{2.23}$$

Moreover, $2j \in \mathbb{Z}_{\geqslant 0}$*, hence*

$$j \in \left\{0, \frac{1}{2}, 1, \frac{3}{2}, \dots\right\}. \tag{2.24}$$

Proof. Since $J_+|\lambda, m_{\max}\rangle = 0$, Lemma 2.12 gives

$$0 = \|J_+|\lambda, m_{\max}\rangle\|^2 = \langle \lambda, m_{\max}|J_- J_+|\lambda, m_{\max}\rangle.$$

Using (2.17) and (2.10),

$$0 = \lambda - \hbar^2 m_{\max}(m_{\max}+1). \tag{2.25}$$

With $j = m_{\max}$ this yields (2.22).

Similarly, from the existence of $m_{\min}$ with $J_-|\lambda, m_{\min}\rangle = 0$ and (2.16), one obtains

$$0 = \|J_-|\lambda, m_{\min}\rangle\|^2 = \lambda - \hbar^2 m_{\min}(m_{\min}-1).$$

Insert $\lambda = \hbar^2 j(j+1)$ and solve for $m_{\min}$; the solutions are $m_{\min} = j+1$ or $m_{\min} = -j$. But $m_{\min} \leqslant m_{\max} = j$, so $m_{\min} = -j$.

Since $J_\pm$ changes m in steps of 1, the set of allowed m values is the integer-spaced ladder from $-j$ to j, giving (2.23). The number of steps from $-j$ to j is $2j$, which must be an integer, proving (2.24). □

Remark 2.15 (Preview: why orbital m is integer). In the *orbital* realization (functions on physical space), single-valuedness under $\phi \mapsto \phi + 2\pi$ forces $m \in \mathbb{Z}$. Here we have not yet chosen a representation, so the algebra alone allows j to be integer or half-integer. The distinction is resolved later by the representation (orbital vs spin).

2.4 Ladder Matrix Elements and Normalization

From Corollary 2.9, we established that applying $J_\pm$ to an eigenstate $|j, m\rangle$ creates a new vector parallel to $|j, m \pm 1\rangle$. However, the algebra alone leaves the *magnitude* of this new vector scaling arbitrary. We now compute the exact proportionality constants in $J_\pm|j, m\rangle \propto |j, m \pm 1\rangle$. This gives the standard ladder matrix elements and fixes normalization conventions.

Theorem 2.16 (Action of $J_\pm$)**.** *For the simultaneous eigenkets* $|j, m\rangle$ *with*

$$J^2|j, m\rangle = \hbar^2 j(j+1)|j, m\rangle, \qquad J_z|j, m\rangle = \hbar m|j, m\rangle,$$

$$J_+|j, m\rangle = \hbar\sqrt{j(j+1) - m(m+1)}\ |j, m+1\rangle, \tag{2.26}$$
$$J_-|j, m\rangle = \hbar\sqrt{j(j+1) - m(m-1)}\ |j, m-1\rangle. \tag{2.27}$$

Proof. By Corollary 2.9, $J_\pm|j, m\rangle$ (if nonzero) is an eigenket of J_z with eigenvalue $\hbar(m \pm 1)$. By Theorem 2.10, it is also an eigenket of J^2 with the same eigenvalue $\hbar^2 j(j+1)$. Hence there exist constants $C_\pm(j, m)$ such that

$$J_\pm|j, m\rangle = \hbar\, C_\pm(j, m)\, |j, m \pm 1\rangle. \tag{2.28}$$

Take norms and use Lemma 2.12:

$$\begin{aligned}\hbar^2|C_+(j,m)|^2 &= \|J_+|j,m\rangle\|^2 = \langle j,m|J_-J_+|j,m\rangle \\ &= \langle j,m|(J^2 - J_z^2 - \hbar J_z)|j,m\rangle = \hbar^2\big(j(j+1) - m(m+1)\big),\end{aligned} \tag{2.29}$$

where we used (2.17). Thus

$$|C_+(j,m)| = \sqrt{j(j+1) - m(m+1)}.$$

Similarly, using (2.16),

$$\begin{aligned}\hbar^2|C_-(j,m)|^2 &= \|J_-|j,m\rangle\|^2 = \langle j,m|J_+J_-|j,m\rangle \\ &= \hbar^2\big(j(j+1) - m(m-1)\big).\end{aligned} \tag{2.30}$$

Finally, one may fix the remaining phase conventions of $|j,m\rangle$ so that $C_\pm(j,m)$ are real and nonnegative, yielding (2.26)–(2.27). □

Corollary 2.17 (Vanishing at the endpoints)**.**

$$J_+|j,j\rangle = 0, \qquad J_-|j,-j\rangle = 0. \tag{2.31}$$

Proof. Insert $m = j$ into (2.26) and $m = -j$ into (2.27). □

3 From Abstract Algebra to Differential Equations

3.1 Representations and Basis Choice

In Section 2 we classified states purely algebraically using operators J_i satisfying (2.1). This produced abstract eigenkets $|j, m\rangle$. The purpose of this section is to explain precisely why differential equations appear only after we choose a concrete *representation*, i.e. a basis in which states are described by functions of continuous variables (like $\mathbf{r}$ or (θ, ϕ)).

Definition 3.1 (Unitary representation of rotations on states)**.** A (strongly continuous) unitary representation of $SO(3)$ on a Hilbert space $\mathcal{H}$ is a map

$$U : SO(3) \to \mathcal{U}(\mathcal{H}), \qquad R \mapsto U(R), \tag{3.1}$$

such that

$$U(R_1 R_2) = U(R_1)U(R_2), \tag{3.2}$$
$$U(I) = I, \tag{3.3}$$
$$U(R)^\dagger U(R) = I. \tag{3.4}$$

Remark 3.2. In quantum mechanics one may allow a *projective* representation (phases may appear). This does not affect the commutator algebra (2.1) nor the ladder-operator spectrum in Section 2. The orbital position-space realization below will correspond to an ordinary (single-valued) representation; spin will require the projective extension.

Definition 3.3 (Change of representation (basis) and wavefunctions)**.** Let $\{|q\rangle\}$ be a generalized basis labelled by a continuous variable q (e.g. $q = \mathbf{r}$ or $q = \Omega = (\theta, \phi)$). The *wavefunction* of $|\psi\rangle \in \mathcal{H}$ in this basis is

$$\psi(q) := \langle q|\psi\rangle. \tag{3.5}$$

An operator A becomes an action on functions via

$$(A\psi)(q) := \langle q|A|\psi\rangle. \tag{3.6}$$

Intuitively, the commutation relations should not change just because we switched languages from kets to functions.

Theorem 3.4 (Commutators are representation-independent)**.** *Let A, B be operators on $\mathcal{H}$, and let $\{|q\rangle\}$ be any basis (discrete or continuous). If $[A, B] = C$ as operators, then in the q-representation the induced actions satisfy*

$$[A, B]\psi \;=\; C\psi \qquad \textit{for all admissible } \psi. \tag{3.7}$$

Proof. For any $|\psi\rangle$,

$$\langle q|([A, B] - C)|\psi\rangle = 0 \quad \text{for all } q.$$

Hence $\langle q|([A, B] - C)|\psi\rangle$ is the zero function, i.e. $([A, B] - C)\psi = 0$ in the representation. □

Remark 3.5 (Why differential operators appear). If q is continuous and the symmetry acts by *moving the label* $q \mapsto q'$, then $U(R)$ acts by composition $\psi(q) \mapsto \psi(q')$. Expanding in small parameters produces derivatives via Taylor expansion. Thus PDEs arise from the *geometric action* of the group on the basis labels, not from additional postulates.

3.2 Position Representation and Translations

We now choose the basis $|\mathbf{r}\rangle$ of (generalized) eigenkets of the position operator $\mathbf{X}$. We impose one physical requirement: *a spatial rotation of the system rotates the position observable as a vector.* This fixes the action of $U(R)$ on $|\mathbf{r}\rangle$ and hence on wavefunctions.

Definition 3.6 (Position operators and eigenkets)**.** Let $\mathbf{X} = (X_1, X_2, X_3)$ be the position operators. The position eigenkets $|\mathbf{r}\rangle$ satisfy

$$\mathbf{X}|\mathbf{r}\rangle = \mathbf{r}\,|\mathbf{r}\rangle, \tag{3.8}$$

and resolve the identity (formally) as

$$\int_{\mathbb{R}^3} d^3r\,|\mathbf{r}\rangle\langle\mathbf{r}| = \mathrm{I}. \tag{3.9}$$

Postulate 3.1 (Position observable under rotations)**.** The unitary $U(R)$ implementing a spatial rotation R satisfies

$$U(R)^\dagger\, X_i\, U(R) = \sum_{j=1}^{3} R_{ij} X_j, \qquad i = 1, 2, 3. \tag{3.10}$$

Equivalently, $U(R)^\dagger\,\mathbf{X}\,U(R) = R\,\mathbf{X}$ as a vector equation.

Justification. Physically, rotating a system by R must rotate the expectation value of its position. For a rotated state $|\psi'\rangle = U(R)|\psi\rangle$, we require $\langle\mathbf{X}\rangle_{\psi'} = R\langle\mathbf{X}\rangle_\psi$. Expanding this expectation value:

$$\langle\psi|U(R)^\dagger\mathbf{X}U(R)|\psi\rangle = \langle\psi|R\mathbf{X}|\psi\rangle.$$

Since this must hold for any state $|\psi\rangle$, the operators must satisfy $U(R)^\dagger\mathbf{X}U(R) = R\mathbf{X}$.

Theorem 3.7 (Rotation maps position eigenkets by rotating their labels)**.** *Under the covariance postulate* (3.10)*,*

$$U(R)\,|\mathbf{r}\rangle = e^{i\alpha(R,\mathbf{r})}\,|R\mathbf{r}\rangle \tag{3.11}$$

for some real phase $\alpha(R, \mathbf{r})$. With a conventional phase choice one may take

$$U(R)\,|\mathbf{r}\rangle = |R\mathbf{r}\rangle. \tag{3.12}$$

Proof. Apply $\mathbf{X}$ to $U(R)|\mathbf{r}\rangle$ and insert the identity $\mathrm{I} = U(R)U(R)^\dagger$ from the left:

$$\mathbf{X}\big(U(R)|\mathbf{r}\rangle\big) = U(R)\,\underbrace{\big(U(R)^\dagger\mathbf{X}U(R)\big)}_{\text{Postulate 3.1}}\,|\mathbf{r}\rangle = U(R)\big(R\mathbf{X}\big)|\mathbf{r}\rangle.$$

Since $\mathbf{X}$ acts on the eigenket $|\mathbf{r}\rangle$, we replace it with the eigenvalue $\mathbf{r}$:

$$= U(R)\big(R\mathbf{r}\big)|\mathbf{r}\rangle = (R\mathbf{r})\,U(R)|\mathbf{r}\rangle.$$

Thus $U(R)|\mathbf{r}\rangle$ is an eigenket of $\mathbf{X}$ with eigenvalue $R\mathbf{r}$. Since the position basis is non-degenerate, $U(R)|\mathbf{r}\rangle$ must be proportional to $|R\mathbf{r}\rangle$. □

With this theorem in hand, we confirm that $U(R)$ physically transports a particle localized at $\mathbf{r} \to R\mathbf{r}$.

Theorem 3.8 (Geometric action on wavefunctions)**.** *In the position representation $\psi(\mathbf{r}) = \langle\mathbf{r}|\psi\rangle$ and with* (3.12)*, the rotated state $|\psi'\rangle := U(R)|\psi\rangle$ has wavefunction*

$$\psi'(\mathbf{r}) = (U(R)\psi)(\mathbf{r}) = \psi(R^{-1}\mathbf{r}). \tag{3.13}$$

Proof. Compute, by the inverse of ((3.12), $\langle r|\, U(R) = \langle R^{-1}\mathbf{r}|$),

$$\psi'(\mathbf{r}) = \langle \mathbf{r}|U(R)|\psi\rangle = \langle U(R)^\dagger \mathbf{r}|\psi\rangle = \langle R^{-1}\mathbf{r}|\psi\rangle = \psi(R^{-1}\mathbf{r}),$$

using $U(R)^\dagger|\mathbf{r}\rangle = |R^{-1}\mathbf{r}\rangle$. □

This theorem tells us that $U(R)$ rotates the wavefunction by looking backward to see where the value came from. To find the value of the new wavefunction, the coordinate lookup must look backward.

Corollary 3.9 (Norm and probability density are rotation-invariant)**.** *Because rotations preserve volume (*$\det R = 1$*),*

$$\int d^3r\, |\psi'(\mathbf{r})|^2 = \int d^3r\, |\psi(R^{-1}\mathbf{r})|^2 = \int d^3r\, |\psi(\mathbf{r})|^2. \tag{3.14}$$

Definition 3.10 (Translation operator on wavefunctions)**.** A spatial translation by $\mathbf{a} \in \mathbb{R}^3$ acts on position-space wavefunctions by

$$\big(U(\mathbf{a})\psi\big)(\mathbf{r}) := \psi(\mathbf{r} - \mathbf{a}). \tag{3.15}$$

Theorem 3.11 (Infinitesimal translations produce a differential generator)**.** *Assuming* $\mathbf{a}$ *is small, the translation operator expands as*

$$U(\mathbf{a}) = I - \frac{i}{\hbar}\,\mathbf{a}\cdot\mathbf{p} + O(\|\mathbf{a}\|^2), \tag{3.16}$$

where the generator $\mathbf{p} = (p_x, p_y, p_z)$ *acts (in the position representation) as*

$$\boxed{\mathbf{p} = -i\hbar\,\nabla.} \tag{3.17}$$

Proof. Taylor expand (3.15):

$$\psi(\mathbf{r} - \mathbf{a}) = \psi(\mathbf{r}) - \mathbf{a}\cdot\nabla\psi(\mathbf{r}) + O(\|\mathbf{a}\|^2). \tag{3.18}$$

By definition of generators for a unitary symmetry,

$$U(\mathbf{a}) = I - \frac{i}{\hbar}\,\mathbf{a}\cdot\mathbf{p} + O(\|\mathbf{a}\|^2).$$

Match the linear terms in $\mathbf{a}$ between this and (3.18) to obtain $\mathbf{p} = -i\hbar\nabla$. □

Corollary 3.12 (Canonical commutation relations in position space)**.** *Let* X_i *act by multiplication:* $(X_i\psi)(\mathbf{r}) = r_i\,\psi(\mathbf{r})$*. Then on a suitable domain (e.g.* $C_0^\infty(\mathbb{R}^3)$*),*

$$[X_i, p_j] = i\hbar\,\delta_{ij}, \qquad [X_i, X_j] = 0, \qquad [p_i, p_j] = 0. \tag{3.19}$$

Proof. Direct calculation using $p_j = -i\hbar\partial_{r_j}$ and multiplication by r_i. □

3.3 Generators and Differential Operators

Equation (3.13) gives the *finite* action of rotations on wavefunctions. We now expand an *infinitesimal* rotation and identify the generator as a differential operator. This is the precise point where derivatives enter, by Taylor expansion of $\psi(R^{-1}\mathbf{r})$.

Definition 3.13 (Infinitesimal rotation parameters)**.** Let $\delta\boldsymbol{\theta} \in \mathbb{R}^3$ be small. The corresponding rotation matrix satisfies

$$R(\delta\boldsymbol{\theta})^{-1}\mathbf{r} = \mathbf{r} - \delta\boldsymbol{\theta}\times\mathbf{r} + O(\|\delta\boldsymbol{\theta}\|^2). \tag{3.20}$$

Theorem 3.14 (Orbital generators are differential operators)**.** *For a spinless particle in the position representation, the rotation generator is*

$$\mathbf{J} \to \mathbf{L} := -i\hbar(\mathbf{r} \times \nabla). \tag{3.21}$$

Equivalently, the infinitesimal action is

$$(U(R(\delta\boldsymbol{\theta}))\psi)(\mathbf{r}) = \psi(\mathbf{r}) - \frac{i}{\hbar}\,\delta\boldsymbol{\theta} \cdot \mathbf{L}\,\psi(\mathbf{r}) + O(\|\delta\boldsymbol{\theta}\|^2). \tag{3.22}$$

Proof. Start from the pullback action (3.13):

$$(U(R)\psi)(\mathbf{r}) = \psi(R^{-1}\mathbf{r}).$$

For $R = R(\delta\boldsymbol{\theta})$, use (3.20) and Taylor expand:

$$\begin{aligned}\psi(R^{-1}\mathbf{r}) &= \psi(\mathbf{r} - \delta\boldsymbol{\theta} \times \mathbf{r}) + O(\delta\theta^2) \\ &= \psi(\mathbf{r}) - (\delta\boldsymbol{\theta} \times \mathbf{r}) \cdot \nabla\psi(\mathbf{r}) + O(\delta\theta^2).\end{aligned} \tag{3.23}$$

Use the scalar triple-product identity

$$(\delta\boldsymbol{\theta} \times \mathbf{r}) \cdot \nabla = \delta\boldsymbol{\theta} \cdot (\mathbf{r} \times \nabla), \tag{3.24}$$

to rewrite (3.23) as

$$(U(R)\psi)(\mathbf{r}) = \psi(\mathbf{r}) - \delta\boldsymbol{\theta} \cdot (\mathbf{r} \times \nabla)\psi(\mathbf{r}) + O(\delta\theta^2).$$

But by definition of the Hermitian generators (Section 1),

$$U(R(\delta\boldsymbol{\theta})) = I - \frac{i}{\hbar}\delta\boldsymbol{\theta} \cdot \mathbf{J} + O(\delta\theta^2).$$

Matching the linear terms in $\delta\boldsymbol{\theta}$ yields $\mathbf{J} \to -i\hbar(\mathbf{r} \times \nabla) = \mathbf{L}$. □

Definition 3.15 (Orbital angular momentum operator)**.** Define

$$\boxed{\mathbf{L} := \mathbf{r} \times \mathbf{p}.} \tag{3.25}$$

In components,

$$L_i := \varepsilon_{ijk}\, X_j\, p_k. \tag{3.26}$$

Theorem 3.16 (Explicit differential form of **L**)**.** *In the position representation,*

$$\boxed{\mathbf{L} = -\,i\hbar\,(\mathbf{r} \times \nabla).} \tag{3.27}$$

Proof. Insert $\mathbf{p} = -i\hbar\nabla$ into (3.25). □

Remark 3.17 (Connection to the abstract algebra). The operators L_i satisfy the same commutator algebra as J_i,

$$[L_i, L_j] = i\hbar\,\varepsilon_{ijk}L_k,$$

so **L** is a concrete realization of the abstract generators **J** on the Hilbert space $L^2(\mathbb{R}^3)$.

3.4 L In Spherical Coordinates

To separate central-potential problems, we need **L** written in variables adapted to spheres: (r, θ, ϕ). Concretely, this will produce:

- $L_z = -i\hbar\,\partial_\phi$ immediately (so m is the Fourier mode in ϕ);
- a closed form for L^2 depending only on θ, ϕ (next subsection).

Spherical Coordinates

Recall

$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta. \tag{3.28}$$

The gradient in spherical coordinates is

$$\nabla = \hat{\mathbf{r}}\,\frac{\partial}{\partial r} + \frac{1}{r}\hat{\boldsymbol{\theta}}\,\frac{\partial}{\partial\theta} + \frac{1}{r\sin\theta}\hat{\boldsymbol{\phi}}\,\frac{\partial}{\partial\phi}. \tag{3.29}$$

(Here $\hat{\mathbf{r}}, \hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\phi}}$ are the usual unit vectors.)

Theorem 3.18 ($L_z = -i\hbar\,\partial_\phi$)**.** *In spherical coordinates,*

$$\boxed{L_z = -i\hbar\,\frac{\partial}{\partial\phi}.} \tag{3.30}$$

Proof. Start from $L_z = xp_y - yp_x = -i\hbar(x\partial_y - y\partial_x)$. Use that $\phi = \arctan(y/x)$ depends only on (x, y) and the chain rule:

$$\frac{\partial}{\partial\phi} = \frac{\partial x}{\partial\phi}\frac{\partial}{\partial x} + \frac{\partial y}{\partial\phi}\frac{\partial}{\partial y} = (-r\sin\theta\sin\phi)\,\partial_x + (r\sin\theta\cos\phi)\,\partial_y = -y\,\partial_x + x\,\partial_y.$$

Therefore $x\partial_y - y\partial_x = \partial_\phi$, hence $L_z = -i\hbar\,\partial_\phi$. □

Theorem 3.19 (Forms of L_x and L_y in spherical coordinates)**.** *In spherical coordinates,*

$$\boxed{L_x = i\hbar\left(\sin\phi\,\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\,\frac{\partial}{\partial\phi}\right)} \tag{3.31}$$

$$\boxed{L_y = i\hbar\left(-\cos\phi\,\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\,\frac{\partial}{\partial\phi}\right).} \tag{3.32}$$

Proof. One route is purely geometric: use $\mathbf{L} = -i\hbar(\mathbf{r}\times\nabla)$ with $\mathbf{r} = r\hat{\mathbf{r}}$ and (3.29). Since $\hat{\mathbf{r}}\times\hat{\mathbf{r}} = 0$,

$$\mathbf{r}\times\nabla = r\hat{\mathbf{r}}\times\left(\hat{\mathbf{r}}\partial_r + \frac{1}{r}\hat{\boldsymbol{\theta}}\partial_\theta + \frac{1}{r\sin\theta}\hat{\boldsymbol{\phi}}\partial_\phi\right) = \hat{\mathbf{r}}\times\hat{\boldsymbol{\theta}}\,\partial_\theta + \frac{1}{\sin\theta}\hat{\mathbf{r}}\times\hat{\boldsymbol{\phi}}\,\partial_\phi.$$

Using $\hat{\mathbf{r}}\times\hat{\boldsymbol{\theta}} = \hat{\boldsymbol{\phi}}$ and $\hat{\mathbf{r}}\times\hat{\boldsymbol{\phi}} = -\hat{\boldsymbol{\theta}}$ gives

$$\mathbf{L} = -i\hbar\left(\hat{\boldsymbol{\phi}}\,\partial_\theta - \frac{1}{\sin\theta}\hat{\boldsymbol{\theta}}\,\partial_\phi\right).$$

Now insert the Cartesian expansions of $\hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\phi}}$:

$$\hat{\boldsymbol{\theta}} = (\cos\theta\cos\phi,\ \cos\theta\sin\phi,\ -\sin\theta),$$
$$\hat{\boldsymbol{\phi}} = (-\sin\phi,\ \cos\phi,\ 0),$$

and read off the x- and y-components. This yields (3.31) and (3.32). □

Remark 3.20 (Ladder Operators). From (3.31)–(3.32), the ladder operators $L_\pm = L_x \pm iL_y$ become

$$L_\pm = \hbar\,e^{\pm i\phi}\left(\pm\frac{\partial}{\partial\theta} + i\cot\theta\,\frac{\partial}{\partial\phi}\right), \tag{3.33}$$

useful for generating $Y_{\ell,m\pm1}$ once $Y_{\ell m}$ is known.

3.5 Derivation of L^2

We want an explicit differential operator for the rotational invariant

$$L^2 = L_x^2 + L_y^2 + L_z^2,$$

in spherical coordinates. The key structural fact is: L^2 *depends only on the angular variables* (θ, ϕ) *and is (up to* $-\hbar^2$*) the Laplacian on the unit sphere.* We derive the standard formula.

Theorem 3.21 (Angular form of L^2)**.** *In spherical coordinates,*

$$\boxed{L^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \, \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right].} \tag{3.34}$$

Proof. We proceed in two steps.

Step 1: Decompose the Laplacian into radial + angular parts. From (3.29), the Laplacian $\nabla^2 = \nabla\cdot\nabla$ in spherical coordinates is

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \, \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right]. \tag{3.35}$$

Define the *angular Laplacian* by

$$\Delta_{S^2} := \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \, \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2}. \tag{3.36}$$

Then (3.35) is

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \Delta_{S^2}. \tag{3.37}$$

Step 2: Identify L^2 with the angular Laplacian. By definition, $\mathbf{L} = -i\hbar(\mathbf{r} \times \nabla)$. To evaluate L^2, we examine the operator product $(\mathbf{r} \times \nabla) \cdot (\mathbf{r} \times \nabla)$. First, we decompose the gradient (3.29) into a radial part and a tangential (angular) part:

$$\nabla = \hat{\mathbf{r}} \, \frac{\partial}{\partial r} + \frac{1}{r} \nabla_{S^2},$$

where ∇_{S^2} contains only θ and ϕ derivatives. When we take the cross product with $\mathbf{r} = r\hat{\mathbf{r}}$, the radial component vanishes because $\hat{\mathbf{r}} \times \hat{\mathbf{r}} = 0$:

$$\mathbf{r} \times \nabla = r\hat{\mathbf{r}} \times \left(\hat{\mathbf{r}} \, \partial_r + \frac{1}{r} \nabla_{S^2} \right) = \hat{\mathbf{r}} \times \nabla_{S^2}.$$

Squaring this operator (taking the dot product with itself) utilizes the vector identity $(\mathbf{A}\times\mathbf{B})\cdot(\mathbf{A}\times\mathbf{B}) = A^2B^2 - (\mathbf{A}\cdot\mathbf{B})^2$. Since $\hat{\mathbf{r}}$ is a unit vector orthogonal to the tangential gradient ∇_{S^2}:

$$(\mathbf{r} \times \nabla) \cdot (\mathbf{r} \times \nabla) = (\hat{\mathbf{r}} \times \nabla_{S^2}) \cdot (\hat{\mathbf{r}} \times \nabla_{S^2}) = \nabla_{S^2} \cdot \nabla_{S^2}. \tag{3.38}$$

This term $\nabla_{S^2} \cdot \nabla_{S^2}$ is precisely the angular Laplacian Δ_{S^2} defined in (3.36). Multiplying by $(-i\hbar)^2 = -\hbar^2$ yields the final result:

$$L^2 = -\hbar^2 \, (\mathbf{r} \times \nabla)^2 = -\hbar^2 \, \Delta_{S^2},$$

which is exactly (3.34). □

Corollary 3.22 (The key separation identity for central potentials)**.** *Combining* (3.37) *and* (3.34)*, we obtain*

$$\boxed{\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{1}{\hbar^2 r^2} \, L^2.} \tag{3.39}$$

Proof. Substitute $\Delta_{S^2} = -(1/\hbar^2)L^2$ from (3.34) into (3.37). □

3.6 Meaning of Spherical Harmonics

Section 2 produced abstract eigenkets $|j, m\rangle$ for J^2, J_z. Section 3.3 produced a concrete realization $J \to L$ as differential operators acting on $\psi(\mathbf{r})$. We now connect these: *spherical harmonics are simply the coordinate representation of the abstract angular-momentum eigenkets.*

Definition 3.23 (Angular basis and spherical harmonics as components)**.** Let $\Omega = (\theta, \phi)$ denote a direction on the unit sphere S^2. Define the angular (direction) basis $|\Omega\rangle$ and the spherical harmonics by

$$Y_{\ell m}(\Omega) \;:=\; \langle \Omega | \ell, m \rangle, \qquad \Omega = (\theta, \phi). \tag{3.40}$$

Remark 3.24 (How $|\Omega\rangle$ is related to $|\mathbf{r}\rangle$)). Heuristically, $|\Omega\rangle$ corresponds to restricting $|\mathbf{r}\rangle$ to a fixed radius and varying direction. More concretely: when $\psi(\mathbf{r}) = \psi(r, \Omega)$ is written in spherical coordinates, the angular dependence lives in functions on S^2 with inner product $\int_{S^2} d\Omega\, (\cdot)^*(\cdot)$.

Theorem 3.25 (Eigenvalue equations become differential equations in the Ω-representation)**.** *In the orbital realization $J \to L$, the abstract eigenvalue relations*

$$J^2 |\ell, m\rangle = \hbar^2 \ell(\ell+1) |\ell, m\rangle, \tag{3.41}$$

$$J_z |\ell, m\rangle = \hbar m\, |\ell, m\rangle \tag{3.42}$$

become, upon taking $\langle \Omega|$,

$$L^2\, Y_{\ell m}(\Omega) = \hbar^2 \ell(\ell+1)\, Y_{\ell m}(\Omega), \tag{3.43}$$

$$L_z\, Y_{\ell m}(\Omega) = \hbar m\, Y_{\ell m}(\Omega). \tag{3.44}$$

In spherical coordinates, L^2 and L_z act as differential operators in (θ, ϕ), so (3.43)–(3.44) *are differential equations whose regular solutions are the spherical harmonics.*

Proof. We derive the differential equation for L^2 explicitly (the L_z case follows identical logic).

Start with the abstract eigenvalue equation for the ket vector, as given in Eq. (3.41):

$$J^2 |\ell, m\rangle = \hbar^2 \ell(\ell+1) |\ell, m\rangle.$$

To convert this into a differential equation, we project the entire equation onto the position (angle) basis by applying the bra $\langle \Omega|$ from the left:

$$\langle \Omega | J^2 | \ell, m \rangle = \langle \Omega | \big(\hbar^2 \ell(\ell+1) |\ell, m\rangle \big).$$

1. The Right-Hand Side (The Scalar): Since the eigenvalue $\hbar^2 \ell(\ell+1)$ is just a complex number, it commutes with the bra and factors out. Using Definition 3.23, we identify the resulting projection as the spherical harmonic function:

$$\text{RHS} = \hbar^2 \ell(\ell+1)\, \underbrace{\langle \Omega | \ell, m \rangle}_{\text{Def. 3.23}} = \hbar^2 \ell(\ell+1) Y_{\ell m}(\Omega).$$

2. The Left-Hand Side (The Operator): We must determine how the abstract operator J^2 acts within the projection. Theorem 3.14 establishes the correspondence between the abstract generator and the differential operator:

$$\mathbf{J} \to \mathbf{L} = -i\hbar(\mathbf{r} \times \nabla).$$

This implies that for any state $|\psi\rangle$, the action of the operator in the position representation is $\langle \mathbf{r} | J | \psi \rangle = L \langle \mathbf{r} | \psi \rangle$. Extending this to the squared operator:

$$\text{LHS} = \langle \Omega | J^2 | \ell, m \rangle = L^2 \langle \Omega | \ell, m \rangle = L^2 Y_{\ell m}(\Omega).$$

Equating the LHS and RHS yields the differential equation:

$$L^2 Y_{\ell m}(\Omega) = \hbar^2 \ell(\ell+1) Y_{\ell m}(\Omega).$$

Applying the same projection to Eq. (3.42) using $J_z \to L_z$ yields the second equation. □

4 Angular Eigenfunctions: Spherical Harmonics

Section 3 produced explicit differential operators L_z and L^2 in spherical coordinates, and Corollary 3.22 gave the key identity splitting ∇^2 into radial and angular parts. We now solve the *angular* eigenvalue problem

$$L^2 Y(\theta,\phi) = \hbar^2 \ell(\ell+1) Y(\theta,\phi), \qquad L_z Y(\theta,\phi) = \hbar m\, Y(\theta,\phi), \tag{4.1}$$

and show that the regular solutions on the sphere are the spherical harmonics $Y_{\ell m}$.

Theorem 4.1 (Central potentials reduce the 3D eigenproblem to an angular eigenproblem + a radial ODE)**.** *Let*

$$H = -\frac{\hbar^2}{2\mu}\nabla^2 + V(r) \tag{4.2}$$

with V depending only on $r = |\mathbf{r}|$. Then

$$[H, L^2] = [H, L_z] = 0. \tag{4.3}$$

Consequently, energy eigenstates may be chosen as simultaneous eigenstates of H, L^2, and L_z, and their angular dependence is fixed by (4.1)*.*

Proof. A rotation leaves r invariant, hence $V(r)$ is rotationally invariant. Since L_i are the generators of rotations in position space, rotational invariance is equivalent to $[V(r), L_i] = 0$ for all i. Also $[p^2, L_i] = 0$ (rotational scalar), hence $[H, L_i] = 0$ for all i, which implies $[H, L^2] = 0$ and $[H, L_z] = 0$. □

4.1 Solve the azimuthal equation

We first solve the simpler eigenvalue equation for L_z, which is already diagonal in ϕ.

Theorem 4.2 (Azimuthal eigenfunctions and quantization of m)**.** *With $L_z = -i\hbar\,\partial_\phi$ (Theorem 3.18), the eigenvalue equation*

$$L_z Y = \hbar m\, Y \tag{4.4}$$

implies that any separable solution $Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$ has

$$\Phi(\phi) = C\, e^{im\phi}. \tag{4.5}$$

Single-valuedness $Y(\theta,\phi+2\pi) = Y(\theta,\phi)$ forces

$$m \in \mathbb{Z}. \tag{4.6}$$

Proof. Insert $Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$ into (4.4):

$$-i\hbar\,\Theta(\theta)\,\Phi'(\phi) = \hbar m\,\Theta(\theta)\,\Phi(\phi) \quad \Rightarrow \quad \Phi'(\phi) = i m\,\Phi(\phi),$$

whose solution is (4.5). Periodicity in ϕ requires $e^{im(\phi+2\pi)} = e^{im\phi}$, hence $e^{i2\pi m} = 1$, i.e. $m \in \mathbb{Z}$. □

4.2 Solution of the Polar Equation

Having determined the azimuthal part $\Phi(\phi) = e^{im\phi}$ (where $m \in \mathbb{Z}$ ensures single-valuedness), we turn our attention to the polar function $\Theta(\theta)$. We start with the L^2 eigenvalue equation, $L^2 Y = \hbar^2 \lambda Y$, and substitute the product form $Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$.

Using the explicit form of L^2 derived in Theorem 3.21:

$$-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\Theta(\theta)\Phi(\phi) = \hbar^2\lambda\,\Theta(\theta)\Phi(\phi).$$

The ϕ-derivative acts only on Φ, giving $\partial_\phi^2 e^{im\phi} = -m^2 e^{im\phi}$. We can then cancel the common factor $-\hbar^2\Phi(\phi)$ (and rearrange signs) to obtain the ordinary differential equation for Θ:

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\,\frac{d\Theta}{d\theta}\right) + \left[\lambda - \frac{m^2}{\sin^2\theta}\right]\Theta(\theta) = 0. \tag{4.7}$$

Change of Variables to $x = \cos\theta$

To solve this ODE, it is standard to switch from the angle θ to the variable $x = \cos\theta$. The domain $\theta \in [0, \pi]$ maps to $x \in [-1, 1]$. The derivatives transform via the chain rule:

$$\frac{d}{d\theta} = \frac{dx}{d\theta}\frac{d}{dx} = -\sin\theta\,\frac{d}{dx}.$$

Substituting this into the differential term of (4.7):

$$\begin{aligned}\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) &= \frac{1}{\sin\theta}\left(-\sin\theta\frac{d}{dx}\right)\left(\sin\theta\left[-\sin\theta\frac{d\Theta}{dx}\right]\right)\\ &= \frac{d}{dx}\left((1-x^2)\frac{d\Theta}{dx}\right),\end{aligned}$$

where we used $\sin^2\theta = 1 - x^2$. The ODE transforms into the Associated Legendre Differential Equation:

$$\frac{d}{dx}\left((1-x^2)\frac{d\Theta}{dx}\right) + \left[\lambda - \frac{m^2}{1-x^2}\right]\Theta = 0. \tag{4.8}$$

Quantization from Regularity

Equation (4.8) has "regular singular points" at the poles $x = \pm 1$ (corresponding to the north and south poles of the sphere). Physically, the wavefunction must be normalizable and finite everywhere, meaning $\Theta(x)$ must not diverge at $x = \pm 1$. This physical requirement is what forces the quantization of λ and constraints on m.

1. Quantization of ℓ (The Series Termination Condition). Consider first the case where $m = 0$ (the standard Legendre equation). We attempt a power series solution $\Theta(x) = \sum_{k=0}^{\infty} c_k x^k$. Substituting this series into the ODE yields a two-term recursion relation for the coefficients:

$$c_{k+2} = \frac{k(k+1) - \lambda}{(k+1)(k+2)}\,c_k.$$

We examine the behavior for large k. As $k \to \infty$, the ratio $c_{k+2}/c_k \to 1$. This behavior is characteristic of the series for $\ln(1 - x^2)$, which diverges to infinity at $x = \pm 1$.

The only way to avoid this divergence is if the series *terminates*—i.e., if c_{k+2} becomes zero for some specific integer $k = \ell$. Looking at the numerator of the recursion, this happens if and only if:

$$\ell(\ell+1) - \lambda = 0 \quad \Longrightarrow \quad \lambda = \ell(\ell+1),$$

where ℓ is a non-negative integer ($\ell = 0, 1, 2, \dots$). This defines the orbital angular momentum quantum number ℓ. The resulting finite polynomials are the Legendre Polynomials, $P_\ell(x)$.

2. Bounds on m (Relationship to Derivatives). For $m \neq 0$, the solutions $P_\ell^m(x)$ are generated by differentiating the Legendre polynomials $|m|$ times. Specifically, they are given by:

$$P_\ell^m(x) \propto (1-x^2)^{|m|/2}\frac{d^{|m|}}{dx^{|m|}}P_\ell(x).$$

Since $P_\ell(x)$ is a polynomial of degree ℓ, differentiating it more than ℓ times yields zero. Therefore, non-vanishing solutions exist only if:

$$|m| \leqslant \ell.$$

If $|m| > \ell$, the wavefunction vanishes identically. This explains why the projection of angular momentum m cannot exceed the total angular momentum ℓ.

Definition 4.3 (Rodrigues formulas)**.** The Legendre polynomials $P_\ell(x)$ are defined by Rodrigues' formula

$$P_\ell(x) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{dx^\ell}(x^2-1)^\ell. \tag{4.9}$$

For $m \geqslant 0$, the associated Legendre polynomials are

$$P_\ell^m(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_\ell(x). \tag{4.10}$$

For $m < 0$ one defines

$$P_\ell^{-m}(x) = (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m(x), \qquad (m>0), \tag{4.11}$$

which ensures a consistent normalization convention later.

4.3 Spherical Harmonics

We now assemble the separated solutions and normalize them to form an orthonormal basis of $L^2(S^2)$.

Definition 4.4 (Spherical harmonics)**.** For $\ell \in \mathbb{Z}_{\geqslant 0}$ and $m \in \mathbb{Z}$ with $|m| \leqslant \ell$, define

$$\boxed{Y_{\ell m}(\theta,\phi) := N_{\ell m} P_\ell^m(\cos\theta)\, e^{im\phi},} \tag{4.12}$$

where P_ℓ^m is as in Definition 4.3 and $N_{\ell m}$ is a real normalization constant.

Theorem 4.5 (Eigenvalue relations)**.** *The spherical harmonics satisfy*

$$L_z Y_{\ell m} = \hbar m\, Y_{\ell m}, \tag{4.13}$$

$$L^2 Y_{\ell m} = \hbar^2 \ell(\ell+1)\, Y_{\ell m}. \tag{4.14}$$

Proof. See Theorem 3.25. $L_z = -i\hbar\partial_\phi$ gives (4.13) immediately from $e^{im\phi}$. Substituting $Y_{\ell m} = \Theta(\theta)e^{im\phi}$ into L^2 (Theorem 3.21) reduces the eigenvalue equation to (4.7) with $\lambda = \ell(\ell+1)$. □

Theorem 4.6 (Orthonormality and normalization constant)**.** *With the inner product on* $L^2(S^2)$*,*

$$\langle f, g\rangle_{S^2} := \int_0^{2\pi}\!\!\int_0^{\pi} f(\theta,\phi)^*\, g(\theta,\phi)\, \sin\theta\, d\theta\, d\phi, \tag{4.15}$$

one can choose

$$\boxed{N_{\ell m} = (-1)^m \sqrt{\frac{2\ell+1}{4\pi}\,\frac{(\ell-m)!}{(\ell+m)!}}} \tag{4.16}$$

(Condon–Shortley convention) so that

$$\int_{S^2} Y_{\ell m}(\Omega)^*\, Y_{\ell' m'}(\Omega)\, d\Omega = \delta_{\ell\ell'}\delta_{mm'}. \tag{4.17}$$

Proof. The ϕ-integral gives

$$\int_0^{2\pi} e^{-im\phi} e^{im'\phi}\, d\phi = 2\pi\,\delta_{mm'}.$$

For fixed m, the polar equation is a Sturm–Liouville problem with weight $\sin\theta$, so eigenfunctions with different ℓ are orthogonal. The standard integral identity for associated Legendre polynomials yields

$$\int_0^{\pi} P_\ell^m(\cos\theta)\, P_{\ell'}^m(\cos\theta)\, \sin\theta\, d\theta = \frac{2(\ell+m)!}{(2\ell+1)(\ell-m)!}\,\delta_{\ell\ell'}.$$

Choosing $N_{\ell m}$ as in (4.16) makes the product of the θ and ϕ integrals equal to $\delta_{\ell\ell'}\delta_{mm'}$. □

Remark 4.7 (Completeness (used implicitly in expansions)). The set $\{Y_{\ell m}\}_{\ell\geqslant 0,\ |m|\leqslant\ell}$ forms a complete orthonormal basis for $L^2(S^2)$. Thus any square-integrable angular function can be expanded in spherical harmonics, which is the angular analogue of a Fourier series.

5 Application: The 3D Hydrogen Atom

5.1 Central Coulomb potential and reduced mass

We now apply the rotation machinery to the hydrogen atom. The key structural points are: (i) the interaction is *central* ($V = V(r)$), so the angular dependence is fixed by L^2, L_z; (ii) the two-body problem reduces to a one-body problem with *reduced mass*.

Definition 5.1 (Coulomb potential)**.** For a nucleus of charge $+Ze$ and an electron of charge $-e$,

$$V(r) = -\frac{Ze^2}{4\pi\varepsilon_0}\,\frac{1}{r} =: -\frac{\kappa Z}{r}, \qquad \kappa := \frac{e^2}{4\pi\varepsilon_0}. \tag{5.1}$$

For hydrogen, $Z = 1$.

Theorem 5.2 (Two-body reduction to one-body Schrödinger equation)**.** *Consider the nonrelativistic two-body Hamiltonian (electron mass m_e, proton mass m_p)*

$$H = \frac{\mathbf{p}_e^2}{2m_e} + \frac{\mathbf{p}_p^2}{2m_p} + V(|\mathbf{r}_e - \mathbf{r}_p|). \tag{5.2}$$

Introduce center-of-mass and relative coordinates

$$\mathbf{R} := \frac{m_e\mathbf{r}_e + m_p\mathbf{r}_p}{m_e + m_p}, \qquad \mathbf{r} := \mathbf{r}_e - \mathbf{r}_p, \tag{5.3}$$

with conjugate momenta $\mathbf{P}$ and $\mathbf{p}$. Then

$$H = \frac{\mathbf{P}^2}{2M} + \left(\frac{\mathbf{p}^2}{2\mu} + V(r)\right), \qquad M := m_e + m_p, \quad \mu := \frac{m_e m_p}{m_e + m_p}. \tag{5.4}$$

Thus the relative wavefunction satisfies a one-body Schrödinger equation with reduced mass μ:

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right)\psi(\mathbf{r}) = E\,\psi(\mathbf{r}). \tag{5.5}$$

Proof. This is a standard linear change of variables. One checks that the kinetic energy decomposes as $\mathbf{p}_e^2/(2m_e) + \mathbf{p}_p^2/(2m_p) = \mathbf{P}^2/(2M) + \mathbf{p}^2/(2\mu)$ and that $V(|\mathbf{r}_e - \mathbf{r}_p|) = V(r)$ depends only on the relative coordinate. The Schrödinger equation then separates into a free center-of-mass part and a relative-coordinate part (5.5). □

5.2 Schrödinger equation in spherical form

We rewrite (5.5) using the angular-momentum operator L^2. This makes the separation into radial and angular pieces transparent.

Using Corollary 3.22,

$$\nabla^2 = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) - \frac{1}{\hbar^2 r^2}L^2. \tag{5.6}$$

Insert (5.6) into (5.5):

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{1}{2\mu r^2}L^2 + V(r)\right]\psi(r,\theta,\phi) = E\,\psi(r,\theta,\phi). \tag{5.7}$$

5.3 Separation of variables

Because $V(r)$ is central, the angular dependence is governed entirely by the eigenvalue problem for L^2 and L_z. We separate variables and reduce (5.7) to a radial ODE.

Let $Y_{\ell m}(\theta, \phi)$ be spherical harmonics (Section 4.3), satisfying

$$L^2 Y_{\ell m} = \hbar^2 \ell(\ell+1) Y_{\ell m}, \qquad L_z Y_{\ell m} = \hbar m Y_{\ell m}. \tag{5.8}$$

Use the separable ansatz

$$\psi(r, \theta, \phi) = R(r)\, Y_{\ell m}(\theta, \phi). \tag{5.9}$$

Substitute (5.9) into (5.7) and use (5.8) to obtain, after dividing by $Y_{\ell m}$,

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) + \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2} R(r) + V(r) R(r) = E\, R(r). \tag{5.10}$$

For the Coulomb potential $V(r) = -\kappa Z/r$, this becomes

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) + \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2} R(r) - \frac{\kappa Z}{r} R(r) = E\, R(r). \tag{5.11}$$

Define the reduced radial function

$$u(r) := r R(r). \tag{5.12}$$

A standard computation yields

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) = \frac{1}{r}\frac{d^2 u}{dr^2}. \tag{5.13}$$

Multiply (5.11) by r and use (5.13) to obtain the 1D-like ODE

$$-\frac{\hbar^2}{2\mu}\frac{d^2 u}{dr^2} + \left[\frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2} - \frac{\kappa Z}{r}\right] u(r) = E\, u(r). \tag{5.14}$$

5.4 Effective potential and centrifugal barrier

Equation (5.14) has the form of a 1D Schrödinger equation on $r \in (0, \infty)$ with an *effective potential*.

Definition 5.3 (Effective potential)**.** Define

$$V_{\text{eff}}(r) := -\frac{\kappa Z}{r} + \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}. \tag{5.15}$$

Then (5.14) is

$$-\frac{\hbar^2}{2\mu} u''(r) + V_{\text{eff}}(r)\, u(r) = E\, u(r). \tag{5.16}$$

Remark 5.4 (Centrifugal barrier). The term

$$\frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2} \tag{5.17}$$

diverges as $r \to 0$ for $\ell \geqslant 1$, suppressing the probability density near the origin. This is the quantum analogue of the classical centrifugal barrier.

5.5 Radial Series Solution and Quantization

We explicitly solve the radial equation (5.14) for bound states ($E < 0$). By factoring out the asymptotic behavior at zero and infinity, we reduce the problem to finding a polynomial solution. The condition that this polynomial must have a finite degree forces the energy to be quantized.

Step 1: Dimensionless Variables and Asymptotics Assume $E < 0$ (bound state). We introduce the wave number k and a dimensionless radial coordinate ρ:

$$k := \frac{\sqrt{-2\mu E}}{\hbar}, \qquad \rho := 2kr. \tag{5.18}$$

Substituting $E = -\hbar^2 k^2/2\mu$ into (5.14) and multiplying by $2\mu/(\hbar^2 k^2)$ transforms the equation into:

$$\frac{d^2u}{d\rho^2} + \left(-\frac{1}{4} + \frac{\eta}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right) u(\rho) = 0, \tag{5.19}$$

where we have defined the dimensionless "Coulomb strength" parameter η:

$$\eta := \frac{\mu\kappa Z}{\hbar^2 k}. \tag{5.20}$$

Step 2: The Ansatz We determine the asymptotic behavior to simplify the equation:

- **As $\rho \to \infty$:** The dominant term is $-1/4$. The equation becomes $u'' - \frac{1}{4}u \approx 0$, yielding $u \sim e^{-\rho/2}$ (the normalizable solution).
- **As $\rho \to 0$:** The centrifugal term dominates. The equation becomes $u'' - \frac{\ell(\ell+1)}{\rho^2}u \approx 0$, yielding regular solution $u \sim \rho^{\ell+1}$.

We therefore look for a solution of the form:

$$u(\rho) = \rho^{\ell+1} e^{-\rho/2} v(\rho). \tag{5.21}$$

Step 3: Differential Equation for $v(\rho)$ Substituting the ansatz (5.21) into (5.19) yields a linear differential equation for $v(\rho)$. The terms involving $\ell(\ell+1)$ cancel exactly, leaving:

$$\rho\frac{d^2v}{d\rho^2} + (2\ell + 2 - \rho)\frac{dv}{d\rho} + (\eta - \ell - 1)v = 0. \tag{5.22}$$

Step 4: The Recurrence Relation We solve for $v(\rho)$ using a power series expansion $v(\rho) = \sum_{j=0}^{\infty} a_j \rho^j$. Substituting this series into (5.22) and collecting powers of ρ^j leads to the recurrence relation:

$$a_{j+1} = \frac{j + \ell + 1 - \eta}{(j+1)(j+2\ell+2)}\, a_j. \tag{5.23}$$

Step 5: Termination Condition (Quantization) For large j, the ratio $a_{j+1}/a_j \approx 1/j$, which implies $v(\rho) \sim e^{\rho}$. This would make the total wavefunction $u(\rho) \sim e^{+\rho/2}$, which is not normalizable. To avoid this divergence, the series must *terminate*. There must exist some non-negative integer n_r (the radial quantum number) such that $a_{n_r} \neq 0$ but $a_{n_r+1} = 0$. From the numerator of (5.23), this requires:

$$n_r + \ell + 1 - \eta = 0.$$

We define the **principal quantum number** n as the integer η:

$$n := n_r + \ell + 1. \tag{5.24}$$

Since $n_r \geqslant 0$ and $\ell \geqslant 0$, the allowed values are $n = 1, 2, 3, \ldots$. This integer constraint determines the energy levels. Using $\eta = n$ in (5.20), we solve for k:

$$k_n = \frac{\mu\kappa Z}{\hbar^2 n}.$$

Substituting k_n back into $E = -\hbar^2 k^2/2\mu$ gives the Bohr energy formula.

Theorem 5.5 (Hydrogenic energy spectrum)**.** *For the Coulomb potential, the bound-state energies depend only on n:*

$$\boxed{E_n = -\frac{\mu(\kappa Z)^2}{2\hbar^2 n^2}.} \tag{5.25}$$

5.6 Closed-form Radial Functions

When the series terminates, the function $v(\rho)$ becomes a polynomial. We identify these as the Associated Laguerre polynomials.

Comparison with Associated Laguerre Equation The standard Associated Laguerre equation for a function $y(x)$ is:

$$xy'' + (\alpha + 1 - x)y' + qy = 0. \tag{5.26}$$

Comparing this to our radial equation (5.22):

$$\rho v'' + (2\ell + 2 - \rho)v' + (n - \ell - 1)v = 0.$$

We see a direct correspondence with $\alpha = 2\ell + 1$ and $q = n - \ell - 1$. Thus, the solutions are proportional to $L_{n-\ell-1}^{2\ell+1}(\rho)$.

Definition 5.6 (Radial Eigenfunctions)**.** Using the Bohr radius $a_0 = \hbar^2/(\mu\kappa)$, the normalized radial wavefunctions are (Shown explicitly in Appendix B):

$$\boxed{R_{n\ell}(r) = \left(\frac{2Z}{na_0}\right)^{3/2} \sqrt{\frac{(n-\ell-1)!}{2n(n+\ell)!}}\, e^{-\rho/2}\, \rho^{\ell}\, L_{n-\ell-1}^{2\ell+1}(\rho),} \tag{5.27}$$

where $\rho = (2Z/na_0)r$.

Remark 5.7 (The Full Wavefunction). The complete position-space eigenstate is the product of this radial part and the spherical harmonic derived in Section 4.2:

$$\psi_{n\ell m}(r, \theta, \phi) = R_{n\ell}(r) Y_{\ell m}(\theta, \phi). \tag{5.28}$$

6 Spin Angular Momentum

In previous chapters, we derived Orbital Angular Momentum (**L**) by considering how rotations affect the *argument* of a wavefunction $\psi(\mathbf{r})$. In this chapter, we derive Spin (**S**) not as an ad-hoc addition, but as a structural necessity arising from the linearity of Quantum Mechanics. We will show that if a particle possesses internal degrees of freedom, the rotation group must act on those degrees of freedom via a unitary representation, inevitably leading to the spin operators and the Lie Algebra of $SU(2)$.

6.1 The Structural Insufficiency of Orbital Angular Momentum

We begin by identifying why $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ is mathematically insufficient to describe all rotational symmetries.

Definition 6.1 (Scalar Wavefunction)**.** A state is called a *scalar wavefunction* if it is a map $\psi : \mathbb{R}^3 \to \mathbb{C}$. The action of a rotation $R \in SO(3)$ on a scalar wavefunction is the geometric pullback:

$$(U_{\text{orb}}(R)\psi)(\mathbf{r}) := \psi(R^{-1}\mathbf{r}). \tag{6.1}$$

Theorem 6.2 (Generator of Scalar Rotations)**.** *The infinitesimal generator of the transformation* (6.1) *is exclusively the orbital angular momentum* **L***.*

Proof. Consider an infinitesimal rotation $R(\boldsymbol{\epsilon})$ by angle $|\boldsymbol{\epsilon}|$ around axis $\hat{\boldsymbol{\epsilon}}$. The coordinate transforms as $R^{-1}\mathbf{r} \approx \mathbf{r} - \boldsymbol{\epsilon} \times \mathbf{r}$. Taylor expanding the wavefunction:

$$\psi(\mathbf{r} - \boldsymbol{\epsilon} \times \mathbf{r}) \approx \psi(\mathbf{r}) - (\boldsymbol{\epsilon} \times \mathbf{r}) \cdot \nabla\psi(\mathbf{r}) = \left(1 - \frac{i}{\hbar}\boldsymbol{\epsilon} \cdot \mathbf{L}\right)\psi(\mathbf{r}).$$

Thus, the unitary operator is generated solely by **L**. □

Remark 6.3 (The Physical Limitation). The assumption that a particle is described by a single complex number at every point in space is a choice, not a law. In classical physics, fields can be vectors (like the Electric field $\mathbf{E}(\mathbf{r})$) or tensors. If a quantum particle has an internal "orientation" or vector nature, we require a more general structure.

6.2 Vector-Valued Wavefunctions and Internal Space

To generalize, we allow the amplitude at a point **r** to be a vector in a finite-dimensional complex vector space.

Definition 6.4 (The Internal Hilbert Space)**.** Let V be a finite-dimensional Hilbert space of dimension d, equipped with an inner product $\langle \cdot, \cdot \rangle_V$. This is the *internal space*. The total Hilbert space of the system is the tensor product:

$$\mathcal{H} = L^2(\mathbb{R}^3) \otimes V. \tag{6.2}$$

Elements of $\mathcal{H}$ are vector-valued wavefunctions $\boldsymbol{\Psi}(\mathbf{r}) = (\psi_1(\mathbf{r}), \ldots, \psi_d(\mathbf{r}))^T$.

Postulate 6.1 (Rotational Invariance of Probability)**.** A spatial rotation R is a symmetry operation. Therefore, it must be represented by a unitary operator $U(R)$ acting on $\mathcal{H}$ that preserves the total probability $\int \boldsymbol{\Psi}^\dagger \boldsymbol{\Psi}\, d^3r$.

Theorem 6.5 (Structure of the Rotation Operator)**.** *The most general local, linear action of a rotation* R *on a state in* $\mathcal{H}$ *decomposes into an external action on* **r** *and an internal action on* V*:*

$$(U(R)\boldsymbol{\Psi})(\mathbf{r}) = D(R)\,\boldsymbol{\Psi}(R^{-1}\mathbf{r}), \tag{6.3}$$

where $D(R)$ *is a* $d \times d$ *unitary matrix acting on* V*.*

Proof. The term $\boldsymbol{\Psi}(R^{-1}\mathbf{r})$ accounts for the relocation of the particle (the coordinate change). However, the vector components inside V might mix among themselves during rotation. Linearity requires this mixing be a matrix multiplication $D(R)$. Unitarity of $U(R)$ implies $D(R)$ must be a unitary matrix ($D^\dagger D = I$) to preserve the norm within V. □

6.3 The Emergence of Spin

We now define Spin rigorously as the generator of the unitary representation $D(R)$.

Definition 6.6 (Spin Operators)**.** Consider an infinitesimal rotation $R(\boldsymbol{\epsilon})$. Since $D(R)$ is unitary and connected to the identity, it can be expanded via a Hermitian generator. We *define* the Spin operator $\mathbf{S}$ by the expansion:

$$D(R(\boldsymbol{\epsilon})) = I - \frac{i}{\hbar}\boldsymbol{\epsilon} \cdot \mathbf{S} + O(\epsilon^2). \tag{6.4}$$

Theorem 6.7 (Additivity of Angular Momenta)**.** *The generator of the total rotation operator $U(R)$ on $\mathcal{H}$ is the sum $\mathbf{J} = \mathbf{L} + \mathbf{S}$.*

Proof. Substitute the infinitesimal forms of both the internal matrix $D(R)$ and the coordinate pullback into Eq. (6.3):

$$\begin{aligned}(U(\epsilon)\boldsymbol{\Psi})(\mathbf{r}) &\approx \left(I - \frac{i}{\hbar}\boldsymbol{\epsilon} \cdot \mathbf{S}\right)\left(\boldsymbol{\Psi}(\mathbf{r}) - \frac{i}{\hbar}(\boldsymbol{\epsilon} \cdot \mathbf{L})\boldsymbol{\Psi}(\mathbf{r})\right) \\ &\approx \left[I - \frac{i}{\hbar}\boldsymbol{\epsilon} \cdot (\mathbf{L} \otimes I + I \otimes \mathbf{S})\right]\boldsymbol{\Psi}(\mathbf{r}).\end{aligned}$$

(Cross terms are order ϵ^2). Thus, the total generator is $\mathbf{J} = \mathbf{L} + \mathbf{S}$. □

Remark 6.8 (Interpretation). Spin is not a distinct physical phenomenon from angular momentum; it is simply the "intrinsic" part of angular momentum that generates rotations on the internal vector index rather than the spatial coordinates.

6.4 The Lie Algebra Constraint

Why must Spin satisfy the same commutation relations as Orbital angular momentum? This is a consequence of the group structure of rotations.

Theorem 6.9 (Homomorphism Property)**.** *For $D(R)$ to represent a rotation, the map $R \mapsto D(R)$ must be a group homomorphism (or a projective representation):*

$$D(R_1)D(R_2) = D(R_1R_2). \tag{6.5}$$

Theorem 6.10 (The Commutator is fixed by Geometry)**.** *The spin operators must satisfy the Lie Algebra of the rotation group:*

$$[S_i, S_j] = i\hbar\epsilon_{ijk}S_k. \tag{6.6}$$

Proof. The commutation relations of generators are determined entirely by the non-commutativity of the group elements near the identity. Geometrically, a rotation of angle ϵ about x followed by y, minus y followed by x, results in a rotation of angle ϵ^2 about z. Since $D(R)$ must track these geometric compositions, the generators S_i must satisfy the same algebra as the geometric generators L_i. (See Chapter 1 for the derivation of the structure constants ϵ_{ijk}). □

6.5 Connection to SU(2)

We now specialize to the simplest non-trivial internal space.

Assumption 6.11. Let the internal space V have the minimal dimension allowed for a non-scalar: $d = 2$. Thus $V \cong \mathbb{C}^2$.

Definition 6.12 (The Group SU(2))**.** The special unitary group $SU(2)$ is the set of 2×2 complex matrices U such that:

1. $U^\dagger U = I$ (Unitarity: preserves probability).

2. $\det(U) = 1$ (Special: volume preserving).

Theorem 6.13 (SU(2) is the Double Cover of SO(3))**.** *There exists a 2-to-1 surjective homomorphism from $SU(2)$ to $SO(3)$. This means that while $SO(3)$ describes rotations of vectors in $\mathbb{R}^3$, $SU(2)$ describes rotations of spinors in $\mathbb{C}^2$. A rotation by 2π corresponds to $-I$ in $SU(2)$, requiring a 4π rotation to return to the identity.*

Remark 6.14. In Quantum Mechanics, states are rays ($|\psi\rangle \sim e^{i\alpha}|\psi\rangle$). Therefore, a representation only needs to hold up to a phase (Projective Representation). This allows fermions to transform under $SU(2)$ rather than just $SO(3)$.

6.6 Pauli Matrices as the Basis of the Algebra

We finally justify why the Pauli matrices appear. They are not arbitrary; they are the necessary mathematical basis for the generator of $SU(2)$.

Theorem 6.15 (The Lie Algebra $\mathfrak{su}(2)$)**.** *The generators (Lie Algebra) of $SU(2)$ are the set of 2×2 matrices X such that $e^{iX} \in SU(2)$. These matrices must be:*

1. ***Hermitian:*** *To ensure U is unitary ($U = e^{-i\epsilon H}$).*
2. ***Traceless:*** *To ensure $\det(U) = 1$. (Recall the identity $\det(e^A) = e^{Tr(A)}$. If $\det = 1$, then $Tr = 0$).*

Theorem 6.16 (Basis Construction)**.** *The vector space of 2×2 traceless Hermitian matrices has dimension 3 over reals. The Pauli matrices form the canonical basis.*

Proof. Let H be an arbitrary 2×2 Hermitian matrix. It has 4 real parameters:

$$H = \begin{pmatrix} a+d & b-ic \\ b+ic & a-d \end{pmatrix}, \quad a,b,c,d \in \mathbb{R}.$$

The condition $\mathrm{Tr}(H) = 0$ implies $(a+d)+(a-d) = 2a = 0$, so $a = 0$. This leaves 3 free parameters (b,c,d). We can expand H as:

$$H = b\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + c\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + d\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

We identify these basis matrices as the Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{6.7}$$

□

Corollary 6.17 (Spin-1/2 Operators)**.** *Since the spin operators S_i must generate $SU(2)$ rotations, they must be proportional to the basis elements σ_i. To satisfy the commutation relation $[S_x, S_y] = i\hbar S_z$ given that $[\sigma_x, \sigma_y] = 2i\sigma_z$, the proportionality constant must be $\hbar/2$.*

$$\boxed{\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}.} \tag{6.8}$$

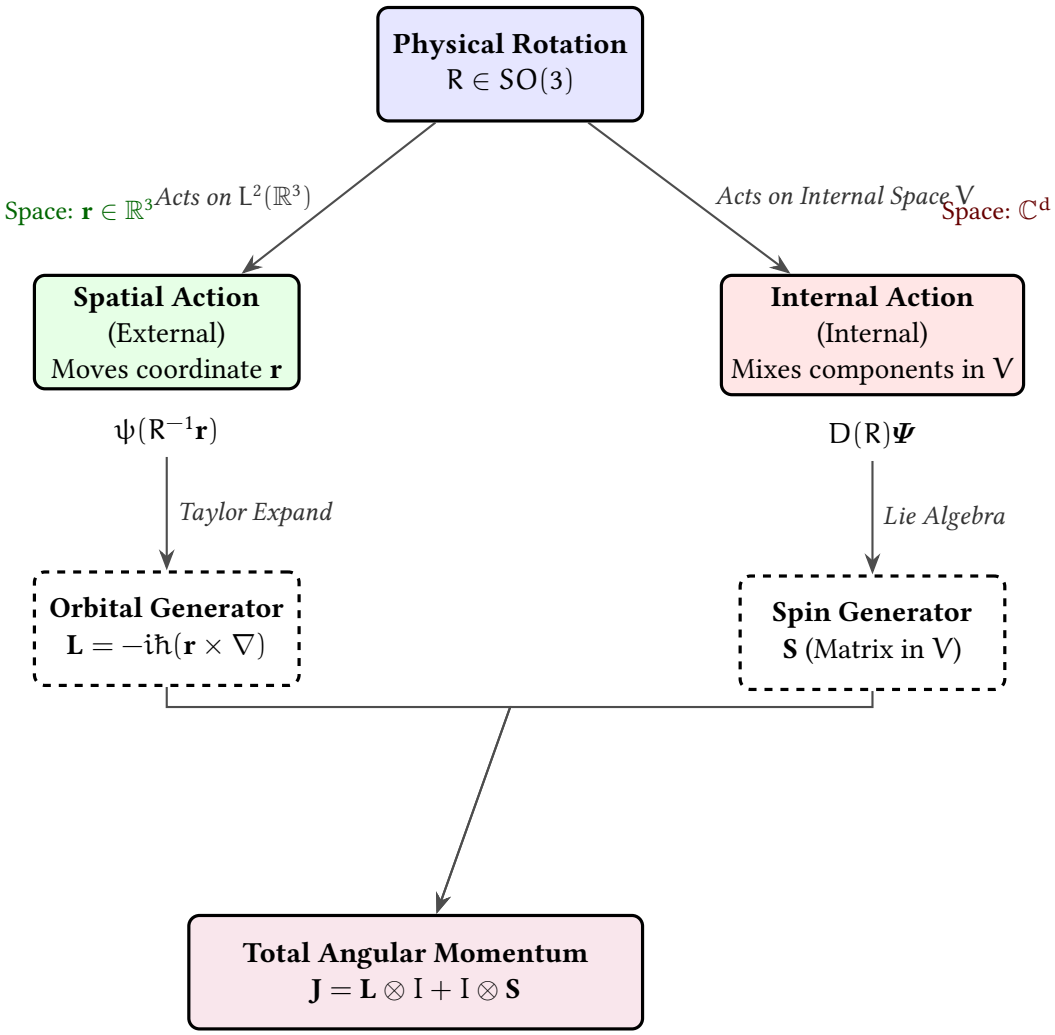

Figure 1: Decomposition of Total Angular Momentum into Orbital and Spin components.

A Derivation of the Ladder Operators

This appendix justifies why this specific linear combination is the natural choice for shifting the eigenvalues of J_z.

The Goal: An Eigen-Operator

We seek an operator, let us call it $\hat{A}$, that transforms an eigenstate of J_z into a new eigenstate with a shifted eigenvalue. Let $|m\rangle$ be an eigenstate such that $J_z|m\rangle = \hbar m|m\rangle$. We require:

$$J_z(\hat{A}|m\rangle) = (m\hbar + \lambda)(\hat{A}|m\rangle) \tag{A.1}$$

where λ is the amount of the shift. Expanding the left side:

$$\begin{aligned} J_z\hat{A}|m\rangle &= (m\hbar + \lambda)\hat{A}|m\rangle \\ (J_z\hat{A} - \hat{A}J_z + \hat{A}J_z)|m\rangle &= m\hbar\hat{A}|m\rangle + \lambda\hat{A}|m\rangle \\ [J_z, \hat{A}]|m\rangle + \hat{A}(\hbar m|m\rangle) &= m\hbar\hat{A}|m\rangle + \lambda\hat{A}|m\rangle \\ [J_z, \hat{A}]|m\rangle &= \lambda\hat{A}|m\rangle \end{aligned}$$

Since this must hold for any state $|m\rangle$, we require the operator relation:

$$[J_z, \hat{A}] = \lambda\hat{A} \tag{A.2}$$

Solving for the Operator

Since J_z commutes with itself and J^2, we look for a solution involving the remaining generators J_x and J_y. Let us propose a linear combination:

$$\hat{A} = \alpha J_x + \beta J_y \tag{A.3}$$

Substituting this into Eq. (A.2) and using the fundamental commutators $[J_z, J_x] = i\hbar J_y$ and $[J_z, J_y] = -i\hbar J_x$:

$$\begin{aligned} [J_z, \alpha J_x + \beta J_y] &= \lambda(\alpha J_x + \beta J_y) \\ \alpha(i\hbar J_y) + \beta(-i\hbar J_x) &= \lambda\alpha J_x + \lambda\beta J_y \end{aligned}$$

Matching the coefficients for the independent operators J_x and J_y:

$$-i\hbar\beta = \lambda\alpha \tag{A.4}$$

$$i\hbar\alpha = \lambda\beta \tag{A.5}$$

Substituting β from Eq. (A.5) into Eq. (A.4):

$$-i\hbar\left(\frac{i\hbar\alpha}{\lambda}\right) = \lambda\alpha \implies \hbar^2\alpha = \lambda^2\alpha \tag{A.6}$$

Assuming $\alpha \neq 0$, we find two possible solutions for the shift amount:

$$\lambda = \pm\hbar \tag{A.7}$$

This proves that the natural "step size" for angular momentum is $\hbar$. Finally, we substitute $\lambda = \pm\hbar$ back into Eq. (A.5) to find the relation between α and β:

$$i\hbar\alpha = (\pm\hbar)\beta \implies \beta = \pm i\alpha$$

Setting the normalization constant $\alpha = 1$, we obtain the two unique solutions:

$$\hat{A}_\pm = J_x \pm iJ_y \tag{A.8}$$

Thus, $J_\pm$ are not arbitrary definitions; they are the unique operators required to shift the J_z eigenvalue by $\pm\hbar$.

B Appendix B: Normalization of the Radial Functions

In this appendix, we explicitly compute the normalization constant for the hydrogenic radial functions $R_{n\ell}(r)$.

The Goal. We seek a constant $N_{n\ell}$ such that the radial function

$$R_{n\ell}(r) = N_{n\ell}\, e^{-\rho/2}\rho^{\ell} L_{n-\ell-1}^{2\ell+1}(\rho), \qquad \text{with } \rho = \left(\frac{2Z}{na_0}\right) r, \tag{B.1}$$

satisfies the normalization condition:

$$\int_0^\infty |R_{n\ell}(r)|^2\, r^2\, dr = 1. \tag{B.2}$$

Step 1: Change of Variables. Substitute Eq. (B.1) into the integral. We change variables from r to the dimensionless variable ρ. From $\rho = \frac{2Z}{na_0} r$, we have:

$$r = \frac{na_0}{2Z}\rho \quad \Longrightarrow \quad dr = \frac{na_0}{2Z} d\rho.$$

The volume element $r^2 dr$ becomes:

$$r^2 dr = \left(\frac{na_0}{2Z}\right)^3 \rho^2 d\rho.$$

Substituting this into Eq. (B.2):

$$1 = |N_{n\ell}|^2 \int_0^\infty \left(e^{-\rho/2}\rho^{\ell} L_{n-\ell-1}^{2\ell+1}(\rho)\right)^2 \left(\frac{na_0}{2Z}\right)^3 \rho^2 d\rho$$
$$1 = |N_{n\ell}|^2 \left(\frac{na_0}{2Z}\right)^3 \int_0^\infty e^{-\rho}\rho^{2\ell+2} \left[L_{n-\ell-1}^{2\ell+1}(\rho)\right]^2 d\rho.$$

Step 2: The Laguerre Integral Identity. Let $q = n - \ell - 1$ and $\alpha = 2\ell + 1$. The integral takes the form:

$$I = \int_0^\infty e^{-\rho}\rho^{\alpha+1} \left[L_q^{\alpha}(\rho)\right]^2 d\rho.$$

Standard orthogonality relations for Laguerre polynomials involve the weight function $e^{-\rho}\rho^{\alpha}$. However, our integrand has an extra factor of ρ (since $\rho^{\alpha+1} = \rho \cdot \rho^{\alpha}$). We use the standard identity for this specific moment:

$$\int_0^\infty e^{-\rho}\rho^{\alpha+1} \left[L_q^{\alpha}(\rho)\right]^2 d\rho = \frac{(q+\alpha)!}{q!}(2q + \alpha + 1). \tag{B.3}$$

Step 3: Calculating the Values. Substitute our specific indices $q = n - \ell - 1$ and $\alpha = 2\ell + 1$ into the identity terms:

- **Factorial term:** $(q + \alpha)! = (n - \ell - 1 + 2\ell + 1)! = (n + \ell)!$.
- **Denominator:** $q! = (n - \ell - 1)!$.
- **Linear term:** $2q + \alpha + 1 = 2(n - \ell - 1) + (2\ell + 1) + 1 = 2n - 2\ell - 2 + 2\ell + 2 = 2n$.

Thus, the value of the integral is:

$$I = \frac{(n + \ell)!}{(n - \ell - 1)!}(2n).$$

Step 4: Solving for $N_{n\ell}$. Substitute the value of I back into the normalization equation:

$$1 = |N_{n\ell}|^2 \left(\frac{n a_0}{2Z}\right)^3 \left[\frac{2n(n+\ell)!}{(n-\ell-1)!}\right].$$

Solving for $|N_{n\ell}|^2$:

$$|N_{n\ell}|^2 = \left(\frac{2Z}{n a_0}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!}.$$

Taking the square root (and choosing the real positive phase convention):

$$N_{n\ell} = \left(\frac{2Z}{n a_0}\right)^{3/2} \sqrt{\frac{(n-\ell-1)!}{2n(n+\ell)!}}. \tag{B.4}$$

This confirms the normalization constant presented in Section 5.6.