Rotation, Spinor, and the Hydrogen Atom

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Abstract

We connect the classical concept of rotation (SO(3)) of column vector $\vec{v} = (v_x, v_y, v_z)^T$ to the quantum mechanical generators of angular momentum ($\vec{L}$). We then introduce spinor ($\psi = \begin{pmatrix}\alpha\\ \beta\end{pmatrix}$) as an intrinsic angular momentum described by fundamental representation of SU(2) & the Pauli matrices. These concepts are applied to explain the spin-orbit coupling & the resulting fine structure observed in the hydrogen atom's spectrum. We thank AI Gemini for helps.

Part 1: From Classical Rotation to Quantum Angular Momentum

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1. Review: Classical Rotation & SO(3)

- **Key Idea:** In classical mechanics, we rotate a vector $\vec{A}$ to a new vector $\vec{v}'$ using a rotation matrix R; $\vec{A}' = R\vec{A}$ which preserving the norm of the vector.
- **2D Example:** Rotation by θ about the z-axis.

$$A'_i = (\mathbf{R}_z(\theta))_{ij} A_j = \begin{pmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{pmatrix}\begin{pmatrix}A_x\\ A_y\end{pmatrix} \Rightarrow \begin{pmatrix}A'_x = A_x cos\theta - A_y sin\theta;\\ A'_x = A_x sin\theta + A_y cos\theta\end{pmatrix} \text{ with } \vec{A}^2 = \vec{A}'^2$$

- **3D Rotations (The Group SO(3)):**
  - Rotations in 3D are defined by an axis $\hat{n}$ and an angle θ.
  - These are 3×3 **orthogonal matrices** ($R^T R = I$) with **determinant = +1**.
  - This group is called **SO(3)**, the "Special Orthogonal Group in 3D."

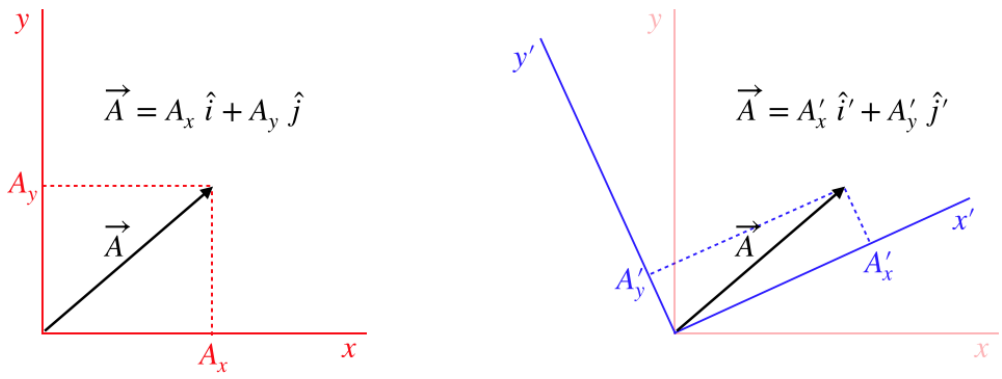

Figure 1: Rotation of vector $\vec{A}$ is equivalent to rotating the frame by the same angle

- **Infinitesimal Rotations:** The key to quantum mechanics is looking at *infinitesimal* rotations.
  - Consider a small rotation $d\theta$ around the z-axis:

$$R_z(d\theta) \approx \begin{pmatrix} 1 & -d\theta & 0 \\ d\theta & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = I - i(d\theta)\begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = I - i(d\theta)G_z$$

  - The matrix G_z is called the **generator** of the rotation.
  - We can find all three generators (in this $j = 1$ representation):

$$G_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad G_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad G_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

2. Quantum Rotations & The Angular Momentum Operator ($\vec{L}$)

- **Key Idea:** In QM, we don't rotate vectors; we rotate the *state vector* $|\psi\rangle$ in Hilbert space. This is done by a **unitary operator** $\hat{U}(R)$.
- **The Rotation Operator:** For a rotation by $\vec{\theta} = \theta\hat{n}$, the operator is:

$$\hat{U}(\vec{\theta}) = e^{-i\vec{\theta}\cdot\vec{\mathcal{J}}/\hbar}$$

  Where $\vec{\mathcal{J}}$ is the **generator of rotations** for the quantum system.
- **Connecting to $\vec{L}$:** For a scalar particle (like a hypothetical spin-0 electron), this generator $\vec{\mathcal{J}}$ is precisely the **orbital angular momentum operator** $\vec{L} = \vec{r} \times \vec{p}$.
- **The Fundamental Algebra (The SO(3) Lie Algebra):**
  - We can check the commutation relations for both the classical generators and the quantum operators.

- Classical Generators: $[G_i, G_j] = i\epsilon_{ijk}G_k$
- Quantum Operators: $[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k$
- **This is the central point.** The commutation relation is the *same*. This algebra *is* the mathematical definition of angular momentum.
- **Angular momentum is the generator of rotations.**

3. Eigenstates of $\vec{L}$ (Spherical Harmonics)

- Because $[\hat{L}^2, \hat{L}_z] = 0$, we can have simultaneous eigenstates $|l, m_l\rangle$.

$$\hat{L}^2|l, m_l\rangle = \hbar^2 l(l+1)|l, m_l\rangle$$
$$\hat{L}_z|l, m_l\rangle = \hbar m_l|l, m_l\rangle$$

- In the position basis, $\langle\theta, \phi|l, m_l\rangle = Y_{lm}(\theta, \phi)$, the Spherical Harmonics.
- **Key Insight:** The Y_{lm}'s are the *basis functions* for the **SO(3)** rotation group. They describe how scalar fields (like the electron's wavefunction) transform under rotation.
- For the Hydrogen atom (ignoring spin), the energy levels E_n are degenerate in l and m_l. This is a direct consequence of the rotational symmetry of the $1/r$ potential.

Part 2: Spin, SU(2), and the Hydrogen Fine Structure

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4. The Problem: Spin-1/2

- **The Experiment: The Stern-Gerlach experiment(1922)**.
  - A beam of silver atoms (which have one outer electron, $l = 0$) is passed through an inhomogeneous magnetic field.
  - Classically (or with just $\vec{L}$), you expect a single continuous blob or an odd number of discrete lines (e.g., $l = 1 \implies m_l = -1, 0, 1 \to 3$ lines).
  - **Result:** The beam split into **two** discrete lines.
- **The Postulate (Uhlenbeck & Goudsmit, 1925):** The electron possesses an *intrinsic* angular momentum, called **spin** ($\vec{S}$), that is not related to its orbital motion.
- This new angular momentum must also be a generator of rotation, so it must obey the *same algebra*:

$$[\hat{S}_i, \hat{S}_j] = i\hbar\epsilon_{ijk}\hat{S}_k$$

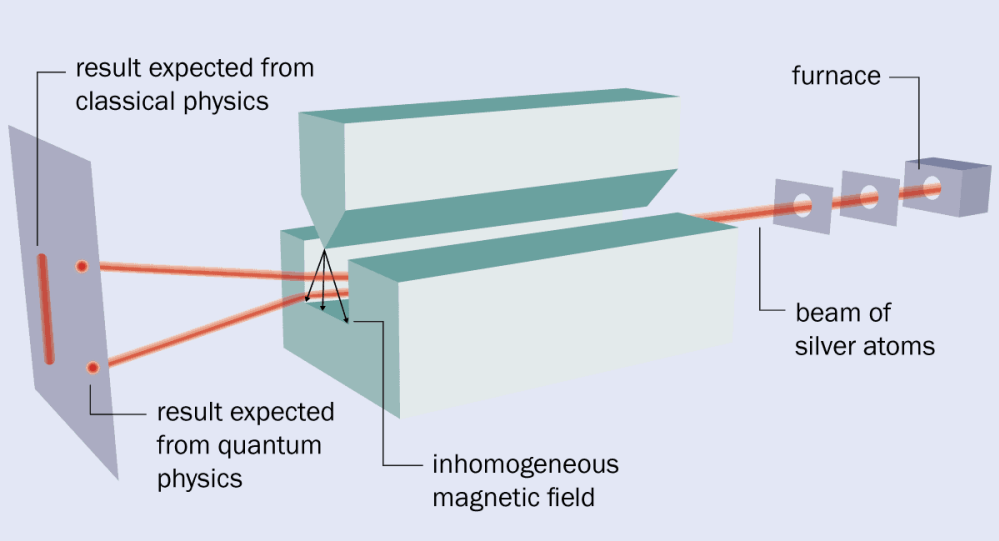

Figure 2: The 1922 Stern-Gerlach experiment demonstrated that a beam of neutral silver atoms, when passed through an inhomogeneous magnetic field, is deflected into two separate beams, not a continuous smear.

- To get 2 lines, we need $2s + 1 = 2$, which implies $s = 1/2$.
- This means the quantum number m_s can be $m_s = -1/2$ ("spin down") or $m_s = +1/2$ ("spin up").

5. The Mathematics of Spin: SU(2) and Spinors

- **Key Idea:** The states are no longer functions. They are abstract vectors in a 2D complex vector space, $\mathbb{C}^2$. We call these objects **spinors**.
  - Spin up: $|\uparrow\rangle = \chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$
  - Spin down: $|\downarrow\rangle = \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$
- The operators $\vec{S}$ that act on these vectors are 2×2 matrices. We can write them as $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$, where $\vec{\sigma}$ are the **Pauli Matrices**:

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

  (One can verify that $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$, which matches the required algebra.)
- **The Rotation Group SU(2):**
  - How do we rotate a spinor? We use the same rotation operator, but with $\vec{S}$ as the generator.

$$\hat{U}(\vec{\theta}) = e^{-i\vec{\theta}\cdot\vec{S}/\hbar} = e^{-i(\vec{\theta}\cdot\vec{\sigma})/2}$$

- This is a 2×2 **unitary matrix** ($U^\dagger U = I$) with **determinant = +1**. This group is called **SU(2)**.

- **Connecting SU(2) to SO(3) (The 720° Twist):**
  - Let's rotate a spinor by 360° (2π) around the z-axis:

$$\hat{U}(2\pi\hat{z}) = e^{-i(2\pi\hat{S}_z)/\hbar} = e^{-i(\pi\sigma_z)} = I\cos(\pi) - i\sigma_z\sin(\pi) = -I$$

$$\hat{U}(2\pi\hat{z})|\uparrow\rangle = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = -\begin{pmatrix} 1 \\ 0 \end{pmatrix} = -|\uparrow\rangle$$

  - **A 360° rotation flips the sign of the spinor!** It does not return to its original state.
  - It takes a **720° (4π) rotation** to get $\hat{U}(4\pi\hat{z}) = (e^{-i\pi\sigma_z})^2 = (-I)^2 = +I$.
  - This is the key difference: **SU(2) is the "double cover" of SO(3).** Spinors are the fundamental objects that rotate under SU(2). Vectors rotate under SO(3).

6. Application: Fine Structure of Hydrogen

- **Total Angular Momentum:** The electron in hydrogen has *both* orbital and spin angular momentum. The total angular momentum is:

$$\vec{J} = \vec{L} + \vec{S}$$

  $\vec{J}$ is the *true* generator of rotations for the *entire* system. The Hamiltonian H will commute with $\vec{J}$, so j and m_j are the good quantum numbers.

- **Spin-Orbit Interaction:**
  - From the electron's frame, the proton orbits it, creating a magnetic field $\vec{B}$.
  - The electron's spin $\vec{S}$ is a magnetic dipole moment $\vec{\mu}_s \propto -\vec{S}$.
  - This leads to an interaction energy (a perturbation) in the Hamiltonian: $\hat{H}_{SO} = -\vec{\mu}_s \cdot \vec{B}$
  - A (non-trivial) derivation shows this is proportional to:

$$\hat{H}_{SO} \propto \frac{1}{r^3}(\vec{L} \cdot \vec{S})$$

- **Evaluating $\vec{L} \cdot \vec{S}$:** We use a classic trick.
  - $\vec{J} = \vec{L} + \vec{S} \implies \hat{J}^2 = (\vec{L} + \vec{S}) \cdot (\vec{L} + \vec{S}) = \hat{L}^2 + \hat{S}^2 + 2\vec{L} \cdot \vec{S}$
  - Therefore: $\vec{L} \cdot \vec{S} = \frac{1}{2}(\hat{J}^2 - \hat{L}^2 - \hat{S}^2)$

- **Splitting the Spectrum:**
  - The unperturbed energy levels depend only on n (e.g., $E_{2s} = E_{2p}$).

- We apply the $\hat{H}_{SO}$ perturbation. The new energy of a state $|n, l, s, j, m_j\rangle$ will be $E_{n,l} + \Delta E_{SO}$.
- The energy shift $\Delta E_{SO} = \langle \hat{H}_{SO} \rangle \propto \langle \vec{L} \cdot \vec{S} \rangle$

$$\langle \vec{L} \cdot \vec{S} \rangle = \frac{\hbar^2}{2}[j(j+1) - l(l+1) - s(s+1)]$$

- **Example: The $n = 2$ Level**
  - **2s state:** $l = 0, s = 1/2$. Only possible total j is $j = 1/2$. (State: $2S_{1/2}$)
  - **2p state:** $l = 1, s = 1/2$. Two possible totals:
    1. $j = l + s = 1 + 1/2 = 3/2$ (State is $2P_{3/2}$)
    2. $j = l - s = 1 - 1/2 = 1/2$ (State is $2P_{1/2}$)
  - The $\vec{L} \cdot \vec{S}$ term is different for these two j values!
  - The $2P_{3/2}$ and $2P_{1/2}$ states, which were degenerate, are now **split** in energy.
  - This splitting is the **fine structure**. (The $2S_{1/2}$ and $2P_{1/2}$ states remain degenerate at this level, but are split by the Lamb shift).

7. Summary & Questions

- Rotation is described by groups: SO(3) for vectors, SU(2) for spinors.
- Angular momentum $(\vec{L}, \vec{S}, \vec{J})$ is the *generator* of these rotations.
- Spin $(\vec{S})$ is a purely quantum form of angular mom. (a "spin-1/2 rep. of SU(2)").
- The physical coupling of $\vec{L}$ and $\vec{S}$ (spin-orbit interaction) breaks the degeneracy of the hydrogen energy levels, giving rise to the **fine structure** we observe in its spectrum.

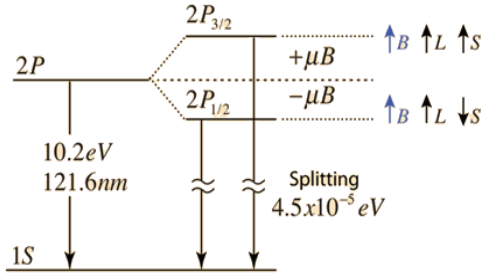

Figure 3: Hydrogen atom $n = 2$ energy levels. The unperturbed level (left) is degenerate. Spin-orbit coupling splits the $2p$ level into two distinct levels, $2P_{3/2}$ and $2P_{1/2}$.