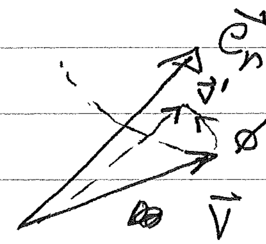
Lecture 9: The Rotation Group

An important symmetry in understanding the structure of matter is the rotation group. Let us begin with a review of the classical theory.

Classical Theory

Rotation in 3D



Axis-angle parametrization

$(\vec{n}, \phi)$ = three parameters : $\begin{cases} 2 \text{ for specifying } \vec{n} \\ \phi \text{ for angle} \end{cases}$

Under a rotation, the coordinates transform as

$$V_i' = \mathbb{R}_{ij} V_j \qquad \text{(repeated index sum convention)}$$

($\mathbb{R}_{ij}$: rotation matrix)

The norm of the vector is preserved $\|\vec{V}'\|^2 = \|\vec{V}\|^2$

$$\Rightarrow \quad V_i' V_i' = V_j V_j = (\mathbb{R}_{ij} V_j)(\mathbb{R}_{ik} V_k)$$

$$\Rightarrow \mathbb{R}_{ij} \mathbb{R}_{ik} = \delta_{jk} \quad \Rightarrow \boxed{\mathbb{R}^T \mathbb{R} = \mathbb{1}}$$

Thus rotation matrices are orthonogonal matrices, i.e. $\mathbb{R}^{-1} = \mathbb{R}^T$

Moreover, a rotation operation preserves the "handedness" of the 3D coordinate system. This translates into $\boxed{\det \mathbb{R} = 1}$

Such det = 1 matrices are said to be "special".

Thus, the group of rotations on 3D vectors is ~~the~~ defined by the set of matrices, 3x3, which are orthogonal and special

$$\boxed{\text{3D rotation group} = SO(3)}$$

The group SO(3) is a Lie group on a 3D manifold. To understand the Lie algebra, consider an infinitesimal rotation, $\delta\phi$

$$\mathbb{R}(\vec{n}, \delta\phi) = \hat{\mathbb{1}} + \delta\phi \hat{A}(\vec{n})$$

← infinitesimal generator

$$\mathbb{R}^T(\vec{n}, \delta\phi)\, \mathbb{R}(\vec{n}\, \delta\phi) = \hat{\mathbb{1}} \Rightarrow \hat{\mathbb{1}} + \delta\phi(\hat{A} + \hat{A}^T) = \hat{\mathbb{1}}$$

$\Rightarrow \boxed{\hat{A} = -\hat{A}^T} \Rightarrow$ The Lie algebra so(3) is the set of anti-symmetric matrices, 3x3

~~Thus~~ A basis for so(3) is $\{\hat{\mathbb{I}}^{(1)}, \hat{\mathbb{I}}^{(2)}, \hat{\mathbb{I}}^{(3)}\}$

$$\hat{\mathbb{I}}^{(1)} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}, \quad \hat{\mathbb{I}}^{(2)} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \quad \hat{\mathbb{I}}^{(3)} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

The Lie algebra basis satisfies the commutators

$$\left[\hat{\mathbb{I}}^{(i)}, \hat{\mathbb{I}}^{(j)}\right] = \epsilon_{ijk}\, \hat{\mathbb{I}}^{(k)}$$

Note: We can also define the algebra with the set of Hermitian matrices with

$$\hat{\mathbb{J}}^{(k)} \equiv -i\, \hat{\mathbb{I}}^{(k)}$$

Then $\left[\hat{\mathbb{J}}^{(i)}, \hat{\mathbb{J}}^{(j)}\right] = i\, \epsilon_{ijk}\, \hat{\mathbb{J}}^{(k)}$

In physics, we tend to use the Hermitian matrices because of there connection to quantum mechanics and observables.

In the axis angle parameterization

$$\mathbb{R}(\vec{n}, \delta\phi) = \hat{\mathbb{1}} + \delta\phi\, \vec{n} \cdot \hat{\vec{\mathbb{I}}}$$

The matrix element of $\hat{\mathbb{I}} = -\epsilon_{ijk}$

$$\Rightarrow \mathbb{R}_{ij}(\vec{n}, \phi)\, V_j = \left(\delta_{ij} + \delta\phi\, \mathbb{I}^{(k)}_{ij}\, n_k\right) V_j$$

$$= \left(\delta_{ij} - \delta\phi\, n_k\, \epsilon_{ijk}\right) V_j$$

$$\Rightarrow \mathbb{R}_{\delta\phi} \vec{V} = \vec{V} + \delta\phi\left(\vec{n} \times \vec{V}\right) \quad \text{as expected}$$

For finite rotation $\boxed{\mathbb{R}(\phi, \vec{n}) = e^{\phi\, \vec{n} \cdot \hat{\vec{\mathbb{I}}}}}$

Quantum Mechanics

Angular momentum operator is the generator of rotations

Infinitesimal: $\hat{U}(\delta\phi) = \hat{\mathbb{1}} - i\,\delta\phi\,\vec{e}_n \cdot \hat{\vec{J}} \qquad (\hbar = 1)$

$$\Rightarrow \hat{U}^{\dagger}(\delta\phi)\,\hat{\vec{V}}\,\hat{U}(\delta\phi) = \hat{\vec{V}} + \delta\phi\,(\vec{e}_n \times \hat{\vec{V}})$$

$$[\hat{J}_i, \hat{V}_j] = i\epsilon_{ijk}\hat{V}_k$$

Finite rotation $\hat{U}(\phi, \vec{e}_n) = e^{-i\phi\,\vec{e}_n \cdot \hat{\vec{J}}}$

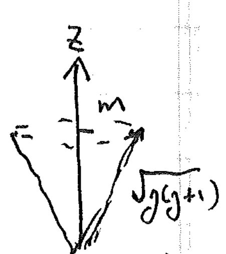
Lie group, Lie algebra of generators

$$[\hat{J}_i, \hat{J}_j] = i\epsilon_{ijk}\hat{J}_k \qquad [\hat{J}^2, \hat{J}_i] = 0$$

Also define spherical basis: $\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y$, $\hat{J}_z$

$$[\hat{J}_+, \hat{J}_-] = 2\hat{J}_z \qquad [\hat{J}_z, \hat{J}_\pm] = \pm\hat{J}_\pm$$

Eigenvalue problem: Simultaneous commuting pair $\{\hat{J}^2, \hat{J}_z\}$



vector picture

$$\hat{J}^2|j,m\rangle = j(j+1)|jm\rangle \qquad \hat{J}_z|j,m\rangle = m|j,m\rangle$$

For given j $\quad -j \le m \le j$ in integer steps

j is half-integer or whole integer

Raising and lowering

$$\hat{J}_\pm|j,m\rangle = \sqrt{j(j+1) \mp m(m\pm 1)}\,|j, m\pm 1\rangle$$

What group are we talking about?
We must be able to accommodate both ½-integer and full-integer j.

Consider $j = \frac{1}{2}$: $\quad \hat{D}^{(\frac{1}{2})}(\phi, \vec{n}) = e^{-i\phi\, \vec{n}\cdot\frac{\hat{\vec{\sigma}}}{2}}$

$$\vec{J} = \vec{S} = \frac{\vec{\sigma}}{2}$$

Consider a sequence of π rotations

$$\hat{D}^{(\frac{1}{2})}(\pi, \vec{n})\, \hat{D}^{(\frac{1}{2})}(\pi, \vec{n}) = e^{-i 2\pi\, \vec{n}\cdot\vec{\sigma}/2}$$

<u>Aside:</u> Recall $e^{-i\frac{\phi}{2}\vec{n}\cdot\vec{\sigma}} = \cos(\frac{\phi}{2})\hat{\mathbb{1}} - i\sin(\frac{\phi}{2})\vec{n}\cdot\hat{\vec{\sigma}}$

$$\Rightarrow e^{-i 2\pi\, \vec{n}\cdot\hat{\vec{\sigma}}/2} = \cos(\tfrac{2\pi}{2})\,\hat{\mathbb{1}} - i\sin(\tfrac{2\pi}{2})\,\vec{n}\cdot\hat{\vec{\sigma}}$$
$$= -\hat{\mathbb{1}}$$

$$\Rightarrow \hat{D}^{(\frac{1}{2})}(\pi, \vec{n})\, \hat{D}^{(\frac{1}{2})}(\pi, \vec{n}) = -\hat{\mathbb{1}} \;!$$

But for $SO(3)$ $\quad \mathbb{R}(\pi, \vec{n})\,\mathbb{R}(\pi, \vec{n}) = \mathbb{R}(2\pi, \hat{n})$
$$= \hat{\mathbb{1}} \;!$$

Thus, the matrices $\hat{D}^{(\frac{1}{2})}(\vec{n}, \phi)$

<u>do not</u> form a representation of $SO(3)$

So for spin angular momentum this is not a representation of SO(3).

The negative sign is an overall phase factor to the wave function which has no physical consequence

$$D^{(\frac{1}{2})}(2\pi)\,|\psi\rangle = -1\,|\psi\rangle \equiv |\psi\rangle$$

So, what group describes rotations in Q.M.?

Consider spin-1/2 $\hat{U}(\vec{n}\phi) = e^{-i\frac{\phi}{2}\hat{\sigma}_n} = \cos\frac{\phi}{2}\hat{\mathbb{1}} - i\sin\frac{\phi}{2}\hat{\sigma}_n$

$$\hat{\sigma}_n = \vec{e}_n \cdot \hat{\vec{\sigma}}$$

Matrix in basis $\{|\pm\rangle_z\}$

$$D^{(\frac{1}{2})} = \begin{bmatrix} \cos\frac{\phi}{2} - i\sin\frac{\phi}{2} n_z & -i\sin\frac{\phi}{2}(n_x - in_y) \\ -i\sin\frac{\phi}{2}(n_x + in_y) & \cos\frac{\phi}{2} + i\sin\frac{\phi}{2} n_z \end{bmatrix}$$

Of the form $D^{(\frac{1}{2})} = \begin{bmatrix} a & b \\ -b^* & a^* \end{bmatrix}$ $\quad |a|^2 + |b|^2 = 1$

$\boxed{\text{Group } 2\times 2 \text{, unitary, } \det = 1 \text{ matrices} \quad SU(2)}$

Loosely speaking SU(2) is like a "doubled" ~~implementation~~ implementation of SO(3).

$$\hat{U}^\dagger(\vec{n}\phi)\,\langle\psi|\hat{\sigma}_i|\psi\rangle\,\hat{U}(\vec{n}\phi) = R_{ij}\,\langle\psi|\sigma_i|\psi\rangle$$

ϕ and $\phi + 2\pi$ yield the same R_{ij}

The rotation group in quantum mechanics is thus SU(2). The matrix representation for $j = 1/2$ is the "defining representation".

The Lie algebra for SU(2) are generated by the spin-1/2 matrices $\vec{S} = \frac{\vec{\sigma}}{2}$

$$\hat{S}_1 = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \hat{S}_2 = \frac{1}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\hat{S}_3 = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

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

The matrices $\hat{D}^{(j)}$ of dim $(2j+1) \times (2j+1)$ form all the possible <u>irreducible representations</u> of SU(2)

- Thus, there is a $j=0$ irrep. This is the trival group with all elements equal to $\mathbb{1}$
- There is a $j=1$ irrep, a $j=\frac{3}{2}$ irrep, etc.

$\boxed{\text{Note: The Lie algebra for SU(2) is the same as the Lie algebra for SO(3)}}$

Both of these manifold look <u>locally</u> the same. But globally they are different (see supplement)

Euler Angle Decomposition

Wigner gave a description for how to calculate the rotation matrices explicitly. Instead of using an axis-angle decomposition, he used an Euler-angle decomposition. As is well known from the classical theory of rigid-body motion, an arbitrary rotation can be written as a sequence of rotations about a space fixed z-axis and y-axis.

$$\hat{D}(\alpha,\beta,\gamma) \equiv \hat{D}_z(\alpha)\,\hat{D}_y(\beta)\,\hat{D}_z(\gamma)$$

Since $\hat{D}_z(\phi)\,|j,m\rangle = e^{-i\phi\hat{J}_z}|j,m\rangle = e^{-im\phi}|j,m\rangle$

$$D^{(j)}_{m'm}(\alpha,\beta,\gamma) = \langle j m'|\,\hat{D}_z(\alpha)\,\hat{D}_y(\beta)\,\hat{D}_z(\gamma)\,|j m\rangle$$

$$= e^{-i(m'\alpha+m\gamma)}\underbrace{\langle j m'|\,e^{-i\beta\hat{J}_y}\,|j m\rangle}_{\equiv\, d^{(j)}_{m'm}}$$

These are known as the "Wigner-d matrices" $\Rightarrow d^{(j)}_{m'm}$ and are tabulated in many places. Once we have the Wigner-d matrices, we can calculate an arbitrary rotation by multiplying the matrix elements by appropriate phases according to the Euler angles α and γ