

# ROTATIONS IN QUANTUM MECHANICS

## Symmetry Overview

Before we delve into specifics of the rotational symmetries, let's review a few general features of all kinds of symmetries: translations, rotations, isospin, whatever, . . . .

- Symmetry transforms of any system — classical quantum, purely mathematical, whatever — always form a *group*: The group product  $S_2S_1$  — the consecutive action of the two transforms, first the  $S_1$  and then the  $S_2$ , is associative,  $S_3(S_2S_1) = (S_3S_2)S_1$ , so we may write it as  $S_3S_2S_1$  without parenthesis. The trivial symmetry transform — making no changes at all — acts as a unity element of the group,  $1S = S1 = S$ . And for any symmetry transform  $S$  there is an inverse transform  $S^{-1}$  such that  $SS^{-1} = S^{-1}S = 1$ .
- The order of the product,  $S_2S_1$  versus  $S_1S_2$  matters in some symmetry groups but not in others. The groups where all symmetries commute,  $S_2S_1 = S_1S_2$ , are called *abelian groups*. Examples:

- \* Group of space translations,  $T(\mathbf{a})T(\mathbf{b}) = T(\mathbf{b})T(\mathbf{a}) = T(\mathbf{a} + \mathbf{b})$ .

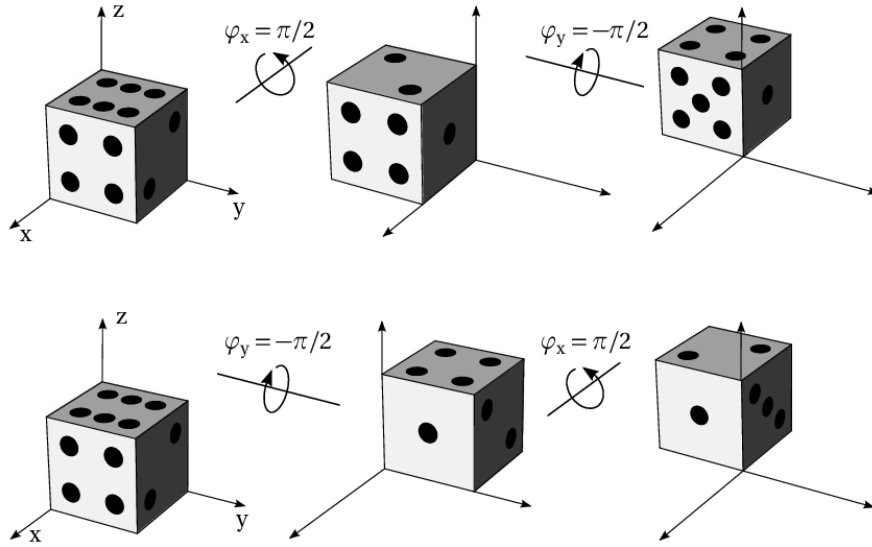
- \* Group of rotations in 2 dimensions,  $R(\alpha)R(\beta) = R(\beta)R(\alpha) = R(\alpha + \beta)$ .

The groups where some symmetries do not commute,  $S_2S_1 \neq S_1S_2$  are called *non-abelian groups*. Example:

- \* Group of rotations in 3 dimensions. Indeed, in 3D rotations around different axis do not commute with each other. Figure 1 on the next page illustrates this fact for

$$R(x \text{ axis}, +90^\circ)R(y \text{ axis}, -90^\circ) \neq R(y \text{ axis}, -90^\circ)R(x \text{ axis}, +90^\circ). \quad (1)$$

- \* Likewise, rotations in any space dimension  $d > 3$  form a non-abelian group.



**Figure 1:** Rotations around different axis do not commute.

- In Quantum Mechanics, the symmetry transforms act as unitary operators  $\hat{U}(S)$  such that

$$\hat{U}(\text{group product } S_2 S_1) = \text{operator product } \hat{U}(S_2) \hat{U}(S_1). \quad (2)$$

Also,  $\hat{U}(1) = 1$  (the unit operator), and

$$\forall S: \quad \hat{U}(S^{-1}) = \hat{U}^{-1}(S) = \hat{U}^\dagger(S). \quad (3)$$

Mathematically speaking, the unitary operators  $\hat{U}(S)$  form a *representation* of the symmetry group. I shall explain this concept later in class.

- Symmetries of a dynamical system must commute with its time evolution: Two states of the system related by a symmetry  $S$  at time  $t_0$  must remain related by the same symmetry at all later times  $t > t_0$ . In Quantum Mechanics, this means that the symmetry operators  $\hat{U}(S)$  must commute with the time evolution operator  $\hat{U}(t - t_0)$ :

$$\begin{aligned} & \text{initial states } |A\rangle \text{ and } |B\rangle = \hat{U}(S) |A\rangle \\ & \text{evolve to } |A'\rangle = \hat{U}(t - t_0) |A\rangle \text{ and } |B'\rangle = \hat{U}(t - t_0) |B\rangle \\ & \text{such that } |B'\rangle = \hat{U}(t - t_0) \hat{U}(S) |A\rangle = \hat{U}(S) \hat{U}(t - t_0) |A\rangle = \hat{U}(S) |A'\rangle. \end{aligned} \quad (4)$$

Consequently, *all the symmetry operators  $\hat{U}(S)$  must commute with the Hamiltonian operator  $\hat{H}$ .*

- For a quantum system with a nonabelian symmetry, this means that the Hamiltonian must commute with symmetry operators which do not commute with each other. As we saw earlier in class, this means that the Hamiltonian's spectrum must be degenerate!
  - \* Example: a particle in a central potential  $V(r)$ . It's Hamiltonian has a non-abelian symmetry of 3D rotations. And as you should have learned in the undergraduate QM class, this Hamiltonian has eigenstates  $|n_r, \ell, m\rangle$  whose energy is degenerate WRT  $m$ ,

$$\hat{H} |n_r, \ell, m\rangle = E(n_r, \ell \text{ only}) |n_r, \ell, m\rangle. \quad (5)$$

- \* For most central potentials, there is no further degeneracy except by accident. But for the Coulomb potential  $V(r) = -\alpha/r$  there is further degeneracy,  $E(n_r, \ell) = E(N = n_r + \ell + 1)$ . Likewise, for a 3D Harmonic oscillator  $V(r) = +\frac{1}{2}m\omega^2 r^2$  we have  $E(n_r, \ell) = E(2n_r + \ell)$ . In both cases, the extra degeneracy is due to a larger symmetry group than just the rotations; we shall return to this point later in class.
- In the *Schrödinger picture* of quantum mechanics, the symmetry operators  $\hat{U}(S)$  act on the quantum states while leaving the operators such as  $\hat{\mathbf{x}}$  or  $\hat{\mathbf{p}}$  invariant,

$$|\psi'\rangle = \hat{U}(S)|\psi\rangle, \quad \langle\psi'| = \langle\psi|\hat{U}^\dagger(S), \quad \hat{A}' = \hat{A}. \quad (6)$$

In the *Heisenberg picture*, the symmetry operators leave the states invariant but act on the operators according to

$$\begin{aligned} |\psi'\rangle &= |\psi\rangle, & \langle\psi'| &= \langle\psi|, \\ \hat{A}' &= \hat{U}^\dagger(S)\hat{A}\hat{U}(S). \end{aligned} \quad (7)$$

But in both pictures, the matrix elements transform in the same way, namely

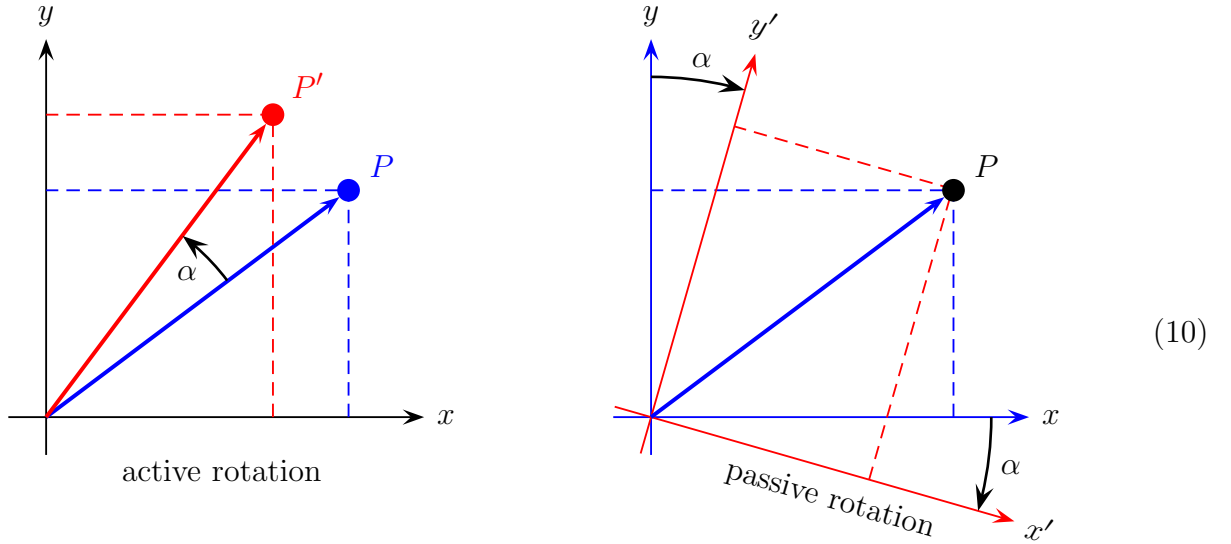
$$\langle\psi_1|\hat{A}|\psi_2\rangle' = \langle\psi_1|\hat{U}^\dagger(S)\hat{A}\hat{U}(S)|\psi_2\rangle. \quad (8)$$

## Rotations in Two Dimensions

In 2 space dimensions there is only one rotation axis, so a rotation can be specified by a single real parameter — the rotation angle  $\alpha$ . A rotation act on components  $(x, y)$  or a position vector  $\mathbf{x}$  — or on components  $(v_x, v_y)$  of any other kind of a vector  $\mathbf{v}$  — as

$$R(\alpha) : \begin{pmatrix} v_x \\ v_y \end{pmatrix} \mapsto \begin{pmatrix} v'_x \\ v'_y \end{pmatrix} = \begin{pmatrix} +\cos \alpha & -\sin \alpha \\ +\sin \alpha & +\cos \alpha \end{pmatrix} \begin{pmatrix} v_x \\ v_y \end{pmatrix}. \quad (9)$$

Note: both active and passive rotations act on components of vectors according to eq. (9), but physically there is a difference: An active rotation rotates bodies — and hence radius-vectors of all their points — in a fixed coordinate frame, while a passive rotation keeps the body where they are while rotating the coordinate axes  $x \rightarrow x'$  and  $y \rightarrow y'$ .



In these notes, I shall henceforth focus on the active rotations.

The 2D rotation group is abelian,  $R(\alpha)R(\beta) = R(\beta)R(\alpha) = R(\alpha + \beta)$ , hence  $R(-\alpha) = R^{-1}(\alpha)$ , so in quantum mechanics the rotations are represented by the unitary operators  $\hat{\mathcal{R}}(\alpha)$  which obey similar product relations,

$$\hat{\mathcal{R}}(\alpha)\hat{\mathcal{R}}(\beta) = \hat{\mathcal{R}}(\beta)\hat{\mathcal{R}}(\alpha) = \hat{\mathcal{R}}(\alpha + \beta), \quad (11)$$

$$\hat{\mathcal{R}}(-\alpha) = \hat{\mathcal{R}}^{-1}(\alpha) = \hat{\mathcal{R}}^\dagger(\alpha). \quad (12)$$

Since any finite rotation obtains as a product of infinite number of infinitesimal rotations,

$$\hat{\mathcal{R}}(\alpha) = \left( \hat{\mathcal{R}}\left(\frac{\alpha}{N}\right) \right)^N, \quad \text{infinitesimal } \frac{\alpha}{N} \text{ for } N \rightarrow \infty, \quad (13)$$

all the rotations obtain by exponentiating a common Hermitian generator

$$\hat{J}_{2d} \stackrel{\text{def}}{=} i\hbar \left. \frac{\partial}{\partial \alpha} \hat{\mathcal{R}}(\alpha) \right|_{\alpha=0}, \quad (14)$$

$$\hat{\mathcal{R}}(\alpha) = \exp\left(\frac{-i\alpha}{\hbar} \hat{J}_{2d}\right). \quad (15)$$

**Proof:** Let's start by checking the Hermiticity of the operator  $\hat{J}_{2d}$  defined according to eq. (14):

$$\begin{aligned} \hat{J}_{2d}^\dagger &= \left( i\hbar \frac{\partial}{\partial \alpha} \hat{\mathcal{R}}(\alpha) \right)^\dagger = -i\hbar \frac{\partial}{\partial \alpha} \hat{\mathcal{R}}^\dagger(\alpha) \\ &\quad \langle\langle \text{using eq. (12)} \rangle\rangle \\ &= -i\hbar \frac{\partial}{\partial \alpha} \hat{\mathcal{R}}(-\alpha) = +i\hbar \frac{\partial}{\partial \alpha} \hat{\mathcal{R}}(\alpha) \\ &= \hat{J}_{2d}. \end{aligned} \quad (16)$$

Next, for an *infinitesimal* angle  $\phi$ , eq. (14) leads to

$$\hat{\mathcal{R}}(\phi) = 1 + \phi \times \left. \frac{\partial}{\partial \phi} \hat{\mathcal{R}}(\phi) \right|_{\phi=0} + O(\phi^2) = 1 + \frac{\phi}{i\hbar} \times \hat{J}_{2d} + O(\phi^2). \quad (17)$$

Now let  $\alpha$  be a finite angle, then in the  $N \rightarrow \infty$  limit  $\phi = \alpha/N$  becomes infinitesimal.

Consequently,

$$\hat{\mathcal{R}}(\alpha/N) = 1 + \frac{\alpha}{Ni\hbar} \times \hat{J}_{2d} + O(\alpha^2/N^2) \quad (18)$$

and therefore

$$\hat{\mathcal{R}}(\alpha) = \left( \hat{\mathcal{R}}(\alpha/N) \right)^N = \left( 1 + \frac{-i(\alpha/\hbar)\hat{J}_{2d}}{N} + O(1/N^2) \right)^N. \quad (19)$$

But

$$\lim_{N \rightarrow \infty} \left( 1 + \frac{A}{N} + O(1/N^2) \right)^N = \exp(A) \quad (20)$$

regardless of the details of the  $O(1/N^2)$  term inside the (), so taking the large  $N$  limit of

eq. (19) gives us

$$\hat{\mathcal{R}}(\alpha) = \exp(-i(\alpha/\hbar)\hat{J}_{2d}), \quad (21)$$

exactly as in eq. (15). *Quod erat demonstrandum.*

We have seen earlier in class that the translations of space symmetries are generated by the net momenta operators  $\hat{P}_x^{\text{net}}$ ,  $\hat{P}_y^{\text{net}}$ , and  $\hat{P}_z^{\text{net}}$ ,

$$\hat{T}(\mathbf{a}) = \exp\left(\frac{-i\mathbf{a} \cdot \mathbf{P}^{\text{net}}}{\hbar}\right). \quad (22)$$

In the same way, *the angular momentum operators generate the rotation symmetries*; in particular, in 2D the operator  $\hat{J}_{2d}$  is the angular momentum operator  $\hat{J}_z^{\text{net}}$  and it generates all the 2D rotation symmetries according to eq. (15).

To see how the operator  $\hat{J}_{2d}$  is the angular momentum operator, let's start with a simple quantum system comprising a single spinless particle. Such particle's quantum state  $|\psi\rangle$  is completely described in terms of its coordinate space wave function  $\psi(x, y)$ , or in polar coordinates

$$\psi(r, \phi) = \langle r, \phi | \psi \rangle. \quad (23)$$

In the polar coordinate basis, the active rotation operators  $\hat{\mathcal{R}}(\alpha)$  act as

$$\hat{\mathcal{R}}(\alpha) |r, \phi\rangle = |r, \phi + \alpha\rangle, \quad (24)$$

hence

$$\hat{\mathcal{R}}^\dagger(\alpha) |r, \phi\rangle = \hat{\mathcal{R}}(-\alpha) |r, \phi\rangle = |r, \phi - \alpha\rangle \quad (25)$$

and therefore

$$\langle r, \phi | \hat{\mathcal{R}}(\alpha) | \psi \rangle = \langle \psi | \hat{\mathcal{R}}^\dagger(\alpha) | r, \phi \rangle^* = \langle \psi | r, \phi - \alpha \rangle^* = \langle r, \phi - \alpha | \psi \rangle. \quad (26)$$

Or in the wave-function terms,

$$\hat{\mathcal{R}}(\alpha)\psi(r, \phi) = \psi(r, \phi - \alpha). \quad (27)$$

Consequently,

$$\hat{J}_{2d}\psi(r, \phi) = i\hbar \left. \frac{\partial}{\partial \alpha} \hat{\mathcal{R}}(\alpha)\psi(r, \phi) \right|_{\alpha=0} = i\hbar \left. \frac{\partial}{\partial \alpha} \psi(r, \phi - \alpha) \right|_{\alpha=0} = -i\hbar \frac{\partial \psi(r, \phi)}{\partial \phi} : \quad (28)$$

in polar coordinates,  $\hat{J}_{2d}$  acts as  $-i\hbar(\partial/\partial\phi)$ . Translating this partial derivative to the Cartesian coordinates, we have

$$\left( \frac{\partial \psi}{\partial \phi} \right)_r = \left( \frac{\partial x}{\partial \phi} \right)_r \times \frac{\partial \psi}{\partial x} + \left( \frac{\partial y}{\partial \phi} \right)_r \times \frac{\partial \psi}{\partial y} = -y \times \frac{\partial \psi}{\partial x} + x \times \frac{\partial \psi}{\partial y}, \quad (29)$$

hence

$$\hat{J}_{2d}\psi(x, y) = +i\hbar y \frac{\partial \psi}{\partial x} - i\hbar x \frac{\partial \psi}{\partial y} = -\hat{y}\hat{p}_x\psi(x, y) + \hat{x}\hat{p}_y\psi(x, y). \quad (30)$$

In other words,

$$\hat{J}_{2d} = -\hat{y}\hat{p}_x + \hat{x}\hat{p}_y = (\hat{\mathbf{x}} \times \hat{\mathbf{p}})_z = \hat{L}_z = \hat{L}_{2d} \quad (31)$$

thus  $\hat{J}_{2d}$  is indeed the 2D orbital angular momentum operator. Or in 3D terms, it's the  $z$  component of the orbital angular momentum, the only component which makes sense for a 2D motion in the  $(x, y)$  plane.

Next, consider a system of two particles described in polar coordinates by  $\psi(r_1, \phi_1; r_2, \phi_2)$ . The rotations move both particles in the  $\phi$  direction, thus

$$\hat{\mathcal{R}}(\alpha) |r_1, \phi_1; r_2, \phi_2\rangle = |r_1, \phi_1 + \alpha; r_2, \phi_2 + \alpha\rangle \quad (32)$$

and hence

$$\hat{\mathcal{R}}(\alpha)\psi(r_1, \phi_1; r_2, \phi_2) = \psi(r_1, \phi_1 - \alpha; r_2, \phi_2 - \alpha). \quad (33)$$

Consequently, taking the derivative WRT  $\alpha$  at  $\alpha = 0$ , we get

$$\hat{J}_{2d}\psi(r_1, \phi_1; r_2, \phi_2) = -i\hbar \left( \frac{\partial}{\partial \phi_1} + \frac{\partial}{\partial \phi_2} \right) \psi(r_1, \phi_1; r_2, \phi_2), \quad (34)$$

or in Cartesian coordinates

$$\hat{J}_{2d}\psi(x_1, y_1; x_2, y_2) = -i\hbar \left( x_1 \frac{\partial \psi}{\partial y_1} - y_1 \frac{\partial \psi}{\partial x_1} + x_2 \frac{\partial \psi}{\partial y_2} - y_2 \frac{\partial \psi}{\partial x_2} \right), \quad (35)$$

hence

$$\hat{J}_{2d} = \hat{x}_1 \hat{p}_{y,1} - \hat{y}_1 \hat{p}_{x,1} + \hat{x}_2 \hat{p}_{y,2} - \hat{y}_2 \hat{p}_{x,2} = \hat{L}_{z,1} + \hat{L}_{z,2} = \hat{L}_z^{\text{net}} = \hat{L}_{2d}^{\text{net}}, \quad (36)$$

the net angular momentum of the two particles.

Likewise, for a system of any number of spinless particles the generator  $\hat{J}$  of the 2D rotation symmetries is the ( $z$  component of) the net angular momentum of all the particles.

Now consider a particle with spin — a degree of freedom unrelated to the space coordinates  $(x, y)$  but subject to non-trivial transformations under rotations. For such a particle

$$\hat{\mathcal{R}}(\alpha) = \hat{\mathcal{R}}_{\text{space}}(\alpha) \times \hat{\mathcal{R}}_{\text{spin}}(\alpha) \quad (37)$$

where the two factors on the RHS commute with each other, hence

$$\hat{J}_{2d} = \hat{L}_{2d} + \hat{S}_{2d}, \quad [\hat{L}_{2d}, \hat{S}_{2d}] = 0. \quad (38)$$

The  $\hat{S}$  operator is called the spinorial angular momentum, or simply *the spin*; we shall see the specific manner of its action later in class. For the moment, let me simply say that if the spin degrees of freedom interact with the particle's motion, then the orbital angular momentum  $\hat{L}$  and the spin  $\hat{S}$  might not be conserved but the net angular momentum  $\hat{J}$  must be conserved,

$$[\hat{L}, \hat{H}] \neq 0, \quad [\hat{S}, \hat{H}] \neq 0, \quad \text{but} \quad [\hat{J}, \hat{H}] = 0. \quad (39)$$

Finally, for a system of several particles with spin, the rotations are generated by the net angular momentum

$$\hat{J}^{\text{net}} = \sum_i^{\text{particles}} (\hat{L}_i + \hat{S}_i), \quad (40)$$

and it is this net angular momentum which should commute with the Hamiltonian  $\hat{H}$ .



## SPECTRUM OF 2D ANGULAR MOMENTUM.

Let's start with the orbital angular momentum  $\hat{L}_{2d}$  of a single particle. Consider an eigenstate  $|\psi\rangle$  of this operator,

$$\hat{L}_{2d} |\psi\rangle = m\hbar |\psi\rangle, \quad (41)$$

where I wrote the eigenvalue as  $m\hbar$  because the angular momentum has the same dimensionality as the  $\hbar$ . In terms of the wave-function  $\psi(r, \phi)$  of the polar coordinates, eq. (41) becomes

$$-i\hbar \frac{\partial \psi}{\partial \phi} = \hbar m \psi \iff \frac{\partial \psi}{\partial \phi} = im\psi, \quad (42)$$

and the general solution of this equation has form

$$\psi(r, \phi) = \psi_r(r) \times e^{im\phi}. \quad (43)$$

However, the polar angle  $\phi$  is a periodic coordinate modulo  $2\pi$ , so any single-valued wave-function must be a periodic function of  $\phi$ ,

$$\psi(r, \phi + 2\pi) = \psi(r, \phi). \quad (44)$$

The solution (43) is periodic with this period if and only if  $m$  is an integer, so the spectrum of  $\hat{L}_{2d}$  comprises

$$L_{2d} = \hbar m, \quad m = 0, \pm 1, \pm 2, \dots \quad (45)$$

Likewise, the spectrum of the net *orbital* angular momentum

$$\hat{L}_{2d}^{\text{net}} = \sum_i^{\text{particles}} \hat{L}_{2d}(i^{\text{th}}) \quad (46)$$

comprises whole numbers in units of  $\hbar$ . This follows from the integer spectrum of each particle's  $\hat{L}_{2d}(i^{\text{th}})$  and the fact that all these individual angular momenta commute with each other.

Another way to get this result is to note that as far as particles' positions  $\mathbf{x}_1, \dots, \mathbf{x}_N$  are concerned, rotating the system through angle  $2\pi$  brings it back to the original position,  $R(2\pi) = 1$  and hence  $\hat{\mathcal{R}}(2\pi)_{\text{space}} = 1$ . In terms of the net orbital angular momentum, this means

$$1 = \hat{\mathcal{R}}(2\pi)_{\text{space}} = \exp\left(\frac{-2\pi i}{\hbar} \hat{L}_{2d}^{\text{net}}\right), \quad (47)$$

thus for any eigenvalue  $\hbar m$  of the  $\hat{L}_{2d}^{\text{net}}$  operator we must have  $\exp(-2\pi i m) = 1$  and hence integer  $m$ .

But the spin part of the angular momentum may have a rather different spectrum. Since the spin degrees of freedom are non-geometrical in nature, rotating them through angle  $2\pi$  does not have to bring them back to the original state. Thus

$$\hat{\mathcal{R}}(2\pi)_{\text{spin}} = \exp\left(\frac{-2\pi i}{\hbar} \hat{S}_{2d}\right) \quad \text{does not have to} = 1, \quad (48)$$

hence the eigenvalues  $\hbar m_s$  of the  $\hat{S}_{2d}$  operator may have non-integer  $m_s$ .

To find the actual spectrum of the 2D spin operator we should distinguish between the quasiparticles which only exist in 2D systems, and the real 3D particles which simply happen to move in only 2 dimensions. For the 3D particles, there is a **theorem**: *a rotation of any system through angle  $4\pi$  around any axis is always trivial*, thus for any quantum system  $\hat{\mathcal{R}}(\text{any axis}, 4\pi) = 1$ . In particular,

$$\hat{\mathcal{R}}(z \text{ axis}, 4\pi)_{\text{spin}} = \exp\left(\frac{-4\pi i}{\hbar} \hat{S}_z\right) = 1, \quad (49)$$

hence for each eigenvalue  $\hbar m_s$  of  $\hat{S}_{2d} = \hat{S}_z$  we must have  $\exp(-4\pi i m_s) = 1$ . Consequently, the allowed values of  $m_s$  are integers and half-integers,

$$m_s = 0, \pm 1, \pm 2, \pm 3, \dots \quad \text{or} \quad m_s = \pm \frac{1}{2}, \pm \frac{3}{2}, \pm \frac{5}{2}, \dots \quad (50)$$

On the other hand, for the purely-2D quasiparticles there is no theorem about rotation by  $4\pi$ , so  $m_s$  does not have to be integer or half-integer but could be some weird fraction. Indeed, the fractional quantum Hall effect is best described in terms of 2D quasiparticles — called *anyons* — with  $m_s = \pm \frac{1}{3}$  or some other fractions.

To understand where the theorem about  $4\pi$  rotations come from, consider a toy model of the spin — the Dirac belt. Let's represent the geometric degrees of freedom of a 2D particle by a pencil lying on a table, and its non-geometric degrees of freedom — the spin — by a belt attached to the pencil and stretching up to the ceiling. As we rotate the pencil by  $2\pi$ , the pencil itself comes back to its original direction, but the belt gets twisted. Similarly, when we rotate the pencil  $n$  times through the  $2\pi$  angle, it comes back to itself, but the belt gets twisted by  $n$  while terms. For a pencil that is stuck on the horizontal plane of the table, these twists cannot be undone without rotating the pencil in the opposite direction, so when we look at the belt as well as the pencil we get  $R(n \times 2\pi) \neq 1$ .

On the other hand, when a pencil is allowed to move up and down, or a belt is allowed to wiggle around the pencil, we cannot undo a rotation by  $2\pi$  but we can undo a rotation by  $4\pi$ , as shown on [this YouTube video](#). Consequently,  $R(4\pi) = 1$ , and that's what restricts the particles' spins to integer or half-integer values.

Another useful general theorem is the **spin-statistics theorem**: for any rotation axis in 3D,  $\hat{R}(2\pi) = \pm 1$  where the sign depends on the particle's statistics: it's  $+1$  for the bosons and  $-1$  for the fermions. Consequently, the bosonic particles have integer spins (in units of  $\hbar$ ) while the fermionic particles have half-integer spins.


There are similar spin-statistics theorems in other dimensions. In  $d \geq 3$  dimensions the only options are bosons with integer spins and fermions with half-integer spins, but in  $d = 2$  dimensions there is a third option: *anyons* with fractional spins and fractional statistics. Instead of

$$\psi(2, 1) = \psi(1, 2) \times \begin{cases} +1 & \text{for the bosons,} \\ -1 & \text{for the fermions,} \end{cases} \quad (51)$$

for the anyons

$$\psi(2, 1) = \psi(1, 2) \times e^{\pm 2\pi i m_s} \quad (52)$$

where the sign of the phase  $\pm 2\pi m_s$  depends on the way we exchange the two particles:



$$\quad (53)$$

## Rotations in Three Dimensions

### ROTATION GROUP.

In 2D there is only one possible axis of rotation, but in 3D one may rotate around any axis one likes. I am going to use unit vectors to indicate the rotation axes, so  $R(\mathbf{n}, \alpha)$  denotes rotating through angle  $\alpha$  around the axis pointed by the unit vector  $\mathbf{n}$ .

A rotation  $R(\mathbf{n}, \delta\alpha)$  through an infinitesimal angle  $\delta\alpha$  acts on a vector  $\mathbf{v}$  as

$$\mathbf{v}' = \mathbf{v} + \delta\alpha \mathbf{n} \times \mathbf{v} + O(\delta\alpha^2). \quad (54)$$

For a finite rotation rotation angle, the action follows from

$$R(\mathbf{n}, \alpha) = \left( R(\mathbf{n}, \frac{\alpha}{N}) \right)^N \quad (55)$$

and taking the  $N \rightarrow \infty$  limit. As you shall see in [homework set#9](#), the finite rotations act as

$$R(\alpha, \mathbf{n}) : \mathbf{v} \mapsto \mathbf{v}' = \cos \alpha \mathbf{v} + \sin \alpha \mathbf{n} \times \mathbf{v} + (1 - \cos \alpha)(\mathbf{n} \cdot \mathbf{v})\mathbf{n}. \quad (56)$$

Or in index notations

$$v'_i = R_{ij}(\mathbf{n}, \alpha)v_j \quad \langle\langle \text{implicit } \sum_j \rangle\rangle, \quad (57)$$

$$\text{for } R_{ij}(\mathbf{n}, \alpha) = \cos \alpha \delta_{ij} + \sin \alpha \epsilon_{ikj}n_k + (1 - \cos \alpha)n_in_j. \quad (58)$$

The 9 coefficients  $R_{ij}(\mathbf{n}, \alpha)$  form a  $3 \times 3$  real matrix  $\|R(\mathbf{n}, \alpha)\|$ ; for example, for  $\mathbf{n} = z$  axis,

$$\|R(z \text{ axis}, \alpha)\| = \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ +\sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (59)$$

You shall also see in the [homework set#9](#) that the matrix  $\|R(\mathbf{n}, \alpha)\|$  of any rotation is a *special orthogonal matrix*, where special means it has a unit determinant  $\det \|R\| = +1$  and

orthogonal means it preserves the magnitudes of the vectors it acts on; orthogonality is the real analogue of the unitarity. In index notations, orthogonality means

$$\begin{aligned}
 v'_i v'_i &= R_{ij} v_j R_{ik} v_k \\
 \text{for } v'_i = R_{ij} v_j : & \quad \parallel \\
 v_j v_j &= \delta_{jk} v_j v_k,
 \end{aligned} \tag{60}$$

which calls for  $R_{ij}R_{ik} = \delta_{jk}$ , or on matrix notations  $\|R\|^\top \|R\| = 1$ . The special orthogonal  $N \times N$  matrices form a group called  $SO(N)$  where the group product is the matrix product. For the present purposes we are interested in the  $SO(3)$  group since any rotation matrix is an  $SO(3)$  matrix. Moreover, the matrix of a product of two consecutive rotations  $R_3 = R_2 R_1$  is the matrix product  $\|R_3\| = \|R_2\| \|R_1\|$ : Indeed, rotating a vector  $\mathbf{v}$  first through  $\alpha_1$  around axis  $\mathbf{n}_1$  and then through  $\alpha_2$  around axis  $\mathbf{n}_2$  produces

$$\begin{aligned}
 v'_j &= R_{jk}^{(1)} v_k, \\
 v''_i &= R_{ij}^{(2)} v'_j = R_{ij}^{(2)} R_{jk}^{(1)} v_k \\
 &= R_{ik}^{(3)} v_k \\
 \text{for } R_{ik}^{(3)} &= R_{ij}^{(2)} R_{jk}^{(1)}, \\
 i. e., \quad \|R_3\| &= \text{matrix product } \|R_2\| \|R_1\|.
 \end{aligned} \tag{61}$$

Finally, any  $SO(3)$  matrix is a rotation matrix  $\|R(\mathbf{n}, \alpha)\|$  for some axis  $\mathbf{n}$  and some angle  $\alpha$ . (Proof is a part of the [homework set#9](#).) Altogether, this means that **the group of 3D rotations is isomorphic to the  $SO(3)$** . In practice, people usually identify the 3D rotation group with the  $SO(3)$  and use the same notation  $R(\mathbf{n}, \alpha)$  for the rotation and for its  $SO(3)$  matrix.

Likewise, the rotation group in any other space dimension  $d \geq 2$  is isomorphic to the  $SO(d)$  and is often identified with the  $SO(d)$ .

## ROTATION GENERATORS

In quantum mechanics, the rotations are represented by the unitary operators  $\hat{\mathcal{R}}(\mathbf{n}, \alpha)$  such that

$$\text{for } R(\mathbf{n}_3, \alpha_3) = R(\mathbf{n}_2, \alpha_2)R(\mathbf{n}_1, \alpha_1) \quad \text{we always have } \hat{\mathcal{R}}(\mathbf{n}_3, \alpha_3) = \hat{\mathcal{R}}(\mathbf{n}_2, \alpha_2)\hat{\mathcal{R}}(\mathbf{n}_1, \alpha_1). \quad (62)$$

Similar to the 2D rotations, the 3D rotations are generated by the angular momentum operator, or rather the 3 components  $\hat{J}_x, \hat{J}_y, \hat{J}_z$  of the 3D angular momentum. To see how this works, consider the infinitesimal rotations

$$R(\mathbf{n}, \delta\alpha) : \mathbf{v} \mapsto \mathbf{v}' = \mathbf{v} + \delta\alpha \mathbf{n} \times \mathbf{v} + O(\delta\alpha^2). \quad (54)$$

To first order in  $\delta\alpha$ , all such rotations commute with each other and the infinitesimal angles — or rather  $\delta\alpha \mathbf{n}$  — add up as vectors:

$$R(\mathbf{n}_3, \delta\alpha_3) = R(\mathbf{n}_2, \delta\alpha_2)R(\mathbf{n}_1, \delta\alpha_1) \quad \text{for } \delta\alpha_3 \mathbf{n}_3 = \delta\alpha_1 \mathbf{n}_1 + \delta\alpha_2 \mathbf{n}_2 + O(\delta\alpha^2). \quad (63)$$

Consequently, for small angles we may treat  $(\alpha n_x, \alpha n_y, \alpha n_z)$  as three components of a vector and take the derivatives of the rotation operator  $\hat{\mathcal{R}}(\mathbf{n}, \alpha) = \hat{\mathcal{R}}(\alpha n_x, \alpha n_y, \alpha n_z)$  with respect to these components. Thus, let

$$\hat{J}_x = i\hbar \frac{\partial \hat{\mathcal{R}}}{\partial(\alpha n_x)}, \quad \hat{J}_y = i\hbar \frac{\partial \hat{\mathcal{R}}}{\partial(\alpha n_y)}, \quad \hat{J}_z = i\hbar \frac{\partial \hat{\mathcal{R}}}{\partial(\alpha n_z)}, \quad \text{all at } \alpha n_x = \alpha n_y = \alpha n_z = 0. \quad (64)$$

Equivalently, we may say that for an infinitesimal rotation angle  $\delta\alpha$

$$\hat{\mathcal{R}}(\mathbf{n}, \delta\alpha) = 1 + \frac{\delta\alpha}{i\hbar} \mathbf{n} \cdot \hat{\mathbf{J}} + O(\delta\alpha^2) \quad (65)$$

where  $\hat{\mathbf{J}}$  is a 3-vector whose components are Hermitian operators  $(\hat{J}_x, \hat{J}_y, \hat{J}_z)$ . As in 2D, the Hermiticity of these operators follows from

$$\hat{\mathcal{R}}^\dagger(\mathbf{n}, \delta\alpha) = \hat{\mathcal{R}}^{-1}(\mathbf{n}, \delta\alpha) = \hat{\mathcal{R}}(\mathbf{n}, -\delta\alpha), \quad (66)$$

hence

$$1 + \frac{\delta\alpha}{-i\hbar} \mathbf{n} \cdot \hat{\mathbf{J}}^\dagger + O(\delta\alpha^2) = 1 + \frac{-\delta\alpha}{i\hbar} \mathbf{n} \cdot \hat{\mathbf{J}} + O(\delta\alpha^2) \quad (67)$$

and therefore  $\hat{\mathbf{J}}^\dagger = \hat{\mathbf{J}}$ .

Similarly to what we had in 2D, eq. (65) for the infinitesimal angles implies that for the finite rotation angles

$$\hat{\mathcal{R}}(\mathbf{n}, \alpha) = \exp\left(\frac{-i\alpha}{\hbar} \mathbf{n} \cdot \hat{\mathbf{J}}\right). \quad (68)$$

Indeed,

$$\begin{aligned} \hat{\mathcal{R}}(\mathbf{n}, \alpha) &= \left(\hat{\mathcal{R}}(\mathbf{n}, \frac{\alpha}{N})\right)^N \\ &\ll \text{for } N \rightarrow \infty \text{ and hence infinitesimal } \frac{\alpha}{n} \gg \\ &= \lim_{N \rightarrow \infty} \left(1 + \frac{\alpha/N}{i\hbar} \mathbf{n} \cdot \hat{\mathbf{J}} + O(\alpha^2/N^2)\right)^N \\ &= \lim_{N \rightarrow \infty} \left(1 + \frac{(\alpha/i\hbar)\mathbf{n} \cdot \hat{\mathbf{J}}}{N} + O(1/N^2)\right)^N \\ &= \exp\left((\alpha/i\hbar)\mathbf{n} \cdot \hat{\mathbf{J}}\right). \end{aligned} \quad (69)$$

Thus, the 3 Hermitian operators  $(\hat{J}_x, \hat{J}_y, \hat{J}_z)$  generate all the rotations of the 3D space.

Physically, these 3 generators are components of the 3D angular momentum operator  $\hat{\mathbf{J}}$ . Indeed, for a single particle without internal degrees of freedom, we may proceed exactly as we did in 2D and show that the  $\hat{J}_z$  operator acts on the wave function  $\psi(x, y, z)$  as  $\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$ . Similarly, we may show that the  $\hat{J}_x$  acts as  $\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$  and  $\hat{J}_y$  acts as  $\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z$ , thus for a single particle without spin  $\hat{\mathbf{J}} = \hat{\mathbf{L}}$ . Likewise, for multiple particles without spin

$$\hat{\mathbf{J}} = \hat{\mathbf{L}}^{\text{net}} = \sum_i^{\text{particles}} \hat{\mathbf{L}}(i^{\text{th}}), \quad (70)$$

and for particles with spins — *i.e.*, internal degrees of freedom that are affected by the space rotations — we have

$$\hat{\mathbf{J}} = \hat{\mathbf{L}}^{\text{net}} + \hat{\mathbf{S}}^{\text{net}} = \sum_i^{\text{particles}} \left(\hat{\mathbf{L}}(i^{\text{th}}) + \hat{\mathbf{S}}(i^{\text{th}})\right). \quad (71)$$

## COMMUTATION RELATIONS

The 3D rotation group  $SO(3)$  is non-abelian, so its generators  $(\hat{J}_x, \hat{J}_y, \hat{J}_z)$  should not commute with each other. Indeed, we know that the orbital angular momenta  $(\hat{L}_x, \hat{L}_y, \hat{L}_z)$  do not commute; instead

$$[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k. \quad (72)$$

Actually, the components of any kind of an angular momentum obey the same commutation relations

$$[\hat{J}_i, \hat{J}_j] = i\hbar\epsilon_{ijk}\hat{J}_k, \quad (73)$$

regardless of its physical origin: The orbital angular momentum, the spin, the angular momentum of the EM fields, the net angular momentum, whatever. Any 3 operators  $(\hat{J}_x, \hat{J}_y, \hat{J}_z)$  that generate 3D rotations of any kind of a quantum system or sub-system must obey the commutation relations (73).

The commutation relations (73) stem from the non-abelian nature of the rotation group  $SO(3)$ . To see how this works, consider two infinitesimal rotations  $R^{(1)} = R(\mathbf{n}_1, \alpha_1)$  and  $R^{(2)} = R(\mathbf{n}_2, \alpha_2)$  to the second order in the infinitesimal angles  $\alpha_1, \alpha_2$ . In index notations

$$\begin{aligned} R_{ij}^{(1)} &= \cos \alpha_1 \delta_{ij} + \sin \alpha_1 \epsilon_{ilj} n_{1l} + (1 - \cos \alpha_1) n_{1i} n_{1j} \\ &= (1 - \frac{1}{2} \alpha_1^2) \delta_{ij} + \alpha_1 \epsilon_{ilj} n_{1l} + \frac{1}{2} \alpha_1^2 n_{1i} n_{1j} + O(\alpha_1^3) \\ &= \delta_{ij} + \alpha_1 \epsilon_{ilj} n_{1l} + \frac{1}{2} \alpha_1^2 (n_{1i} n_{1j} - \delta_{ij}) + O(\alpha_1^3) \end{aligned} \quad (74)$$

and likewise

$$R_{jk}^{(2)} = \delta_{jk} + \alpha_2 \epsilon_{jmk} n_{2m} + \frac{1}{2} \alpha_2^2 (n_{2j} n_{2k} - \delta_{jk}) + O(\alpha_2^3). \quad (75)$$

Now consider the products of these two rotations matrices in both orders:

$$\begin{aligned} (R^{(1)} R^{(2)})_{ik} &= R_{ij}^{(1)} R_{jk}^{(2)} \\ &= \delta_{ij} \times \delta_{jk} + \alpha_1 \epsilon_{ilj} n_{1l} \times \delta_{jk} + \delta_{ij} \times \alpha_2 \epsilon_{jmk} n_{2m} \\ &\quad + \frac{1}{2} \alpha_1^2 (n_{1i} n_{1j} - \delta_{ij}) \times \delta_{jk} + \delta_{ij} \times \frac{1}{2} \alpha_2^2 (n_{2j} n_{2k} - \delta_{jk}) \\ &\quad + \alpha_1 \epsilon_{ilj} n_{1l} \times \alpha_2 \epsilon_{jmk} n_{2m} + O(\alpha^3) \end{aligned} \quad (76)$$



$$\begin{aligned}
&= \delta_{ik} + (\alpha_1 n_{i\ell} + \alpha_2 n_{2\ell}) \epsilon_{i\ell k} + \frac{1}{2} \alpha_1^2 (n_{1i} n_{1k} - \delta_{ik}) + \frac{1}{2} \alpha_2^2 (n_{2i} n_{2k} - \delta_{ik}) \\
&\quad + \alpha_1 \alpha_2 \epsilon_{i\ell j} \epsilon_{jmk} \times n_{1\ell} n_{2m} + O(\alpha^3),
\end{aligned} \tag{76}$$

and likewise

$$\begin{aligned}
(R^{(2)} R^{(1)})_{ik} &= R_{ij}^{(2)} R_{jk}^{(1)} \\
&= \delta_{ik} + (\alpha_1 n_{i\ell} + \alpha_2 n_{2\ell}) \epsilon_{i\ell k} + \frac{1}{2} \alpha_1^2 (n_{1i} n_{1k} - \delta_{ik}) + \frac{1}{2} \alpha_2^2 (n_{2i} n_{2k} - \delta_{ik}) \\
&\quad + \alpha_1 \alpha_2 \epsilon_{i\ell j} \epsilon_{jmk} \times n_{2\ell} n_{1m} + O(\alpha^3).
\end{aligned} \tag{77}$$

Note the difference between the terms marked in red. Thus, to the second order in the infinitesimal angles

$$(R^{(1)} R^{(2)} - R^{(2)} R^{(1)})_{ik} = \alpha_1 \alpha_2 \epsilon_{i\ell j} \epsilon_{jmk} (n_{1\ell} n_{2m} - n_{2\ell} n_{1m}) + O(\alpha^3) \tag{78}$$

where

$$\begin{aligned}
\epsilon_{i\ell j} \epsilon_{jmk} (n_{1\ell} n_{2m} - n_{2\ell} n_{1m}) &= (\delta_{im} \delta_{\ell k} - \delta_{ik} \delta_{\ell m}) (n_{1\ell} n_{2m} - n_{2\ell} n_{1m}) \\
&= n_{1k} n_{2i} - \delta_{ik} (\mathbf{n}_1 \cdot \mathbf{n}_2) - n_{2k} n_{1i} + \delta_{ik} (\mathbf{n}_2 \cdot \mathbf{n}_1) \\
&= n_{1k} n_{2i} - n_{1i} n_{2k} = (-\delta_{i\ell} \delta_{km} + \delta_{im} \delta_{k\ell}) n_{1\ell} n_{2m} \\
&= -\epsilon_{ikj} \epsilon_{j\ell m} n_{i\ell} n_{2m} = -\epsilon_{ikj} (\mathbf{n}_1 \times \mathbf{n}_2)_j \\
&= +\epsilon_{ijk} (\mathbf{n}_1 \times \mathbf{n}_2)_j.
\end{aligned} \tag{79}$$

Consequently,

$$(R^{(1)} R^{(2)} - R^{(2)} R^{(1)})_{ik} = \epsilon_{ijk} (\alpha_1 \alpha_2 \mathbf{n}_1 \times \mathbf{n}_2)_j + O(\alpha_{1,2}^3) = (R^{(3)} - 1)_{ik} + O(\alpha_{1,2}^3) \tag{80}$$

for

$$R^{(3)} = R(\mathbf{n}_3, \alpha_3), \quad \alpha_3 \mathbf{n}_3 = \alpha_1 \alpha_2 (\mathbf{n}_1 \times \mathbf{n}_2). \tag{81}$$

The operators  $\hat{\mathcal{R}}(\mathbf{n}, \alpha)$  representing rotations in the Hilbert space of any quantum system

should obey similar commutation relation: for infinitesimal angles  $\alpha_1$  and  $\alpha_2$ ,

$$\hat{\mathcal{R}}(\mathbf{n}_1, \alpha_1)\hat{\mathcal{R}}(\mathbf{n}_2, \alpha_2) - \hat{\mathcal{R}}(\mathbf{n}_2, \alpha_2)\hat{\mathcal{R}}(\mathbf{n}_1, \alpha_1) = \hat{\mathcal{R}}(\mathbf{n}_3, \alpha_3) - 1 + O(\alpha_{1,2}^3) \quad (82)$$

$$\text{for } \alpha_3\mathbf{n}_3 = \alpha_1\alpha_2(\mathbf{n}_1 \times \mathbf{n}_2). \quad (83)$$

On the other hand,

$$\hat{\mathcal{R}}(\mathbf{n}, \alpha) = \exp\left(\frac{-i\alpha}{\hbar}\mathbf{n} \cdot \hat{\mathbf{J}}\right) = 1 - \frac{i\alpha}{\hbar}(\mathbf{n} \cdot \hat{\mathbf{J}}) - \frac{\alpha^2}{2\hbar^2}(\mathbf{n} \cdot \hat{\mathbf{J}})^2 + O(\alpha^3), \quad (84)$$

hence

$$\begin{aligned} \hat{\mathcal{R}}(\mathbf{n}_1, \alpha_1)\hat{\mathcal{R}}(\mathbf{n}_2, \alpha_2) &= 1 - \frac{i\alpha_1}{\hbar}(\mathbf{n}_1 \cdot \hat{\mathbf{J}}) - \frac{i\alpha_2}{\hbar}(\mathbf{n}_2 \cdot \hat{\mathbf{J}}) \\ &\quad - \frac{\alpha_1^2}{2\hbar^2}(\mathbf{n}_1 \cdot \hat{\mathbf{J}})^2 - \frac{\alpha_2^2}{2\hbar^2}(\mathbf{n}_2 \cdot \hat{\mathbf{J}})^2 \\ &\quad - \frac{\alpha_1\alpha_2}{\hbar^2}(\mathbf{n}_1 \cdot \hat{\mathbf{J}})(\mathbf{n}_2 \cdot \hat{\mathbf{J}}) + O(\alpha_{1,2}^3) \end{aligned} \quad (85)$$

and likewise

$$\begin{aligned} \hat{\mathcal{R}}(\mathbf{n}_2, \alpha_2)\hat{\mathcal{R}}(\mathbf{n}_1, \alpha_1) &= 1 - \frac{i\alpha_1}{\hbar}(\mathbf{n}_1 \cdot \hat{\mathbf{J}}) - \frac{i\alpha_2}{\hbar}(\mathbf{n}_2 \cdot \hat{\mathbf{J}}) \\ &\quad - \frac{\alpha_1^2}{2\hbar^2}(\mathbf{n}_1 \cdot \hat{\mathbf{J}})^2 - \frac{\alpha_2^2}{2\hbar^2}(\mathbf{n}_2 \cdot \hat{\mathbf{J}})^2 \\ &\quad - \frac{\alpha_2\alpha_1}{\hbar^2}(\mathbf{n}_2 \cdot \hat{\mathbf{J}})(\mathbf{n}_1 \cdot \hat{\mathbf{J}}) + O(\alpha_{1,2}^3). \end{aligned} \quad (86)$$

Again, the red color marks the terms different between the two products. Taking the difference, we arrive at

$$[\hat{\mathcal{R}}(\mathbf{n}_1, \alpha_1), \hat{\mathcal{R}}(\mathbf{n}_2, \alpha_2)] = -\frac{\alpha_1\alpha_2}{\hbar^2}[(\mathbf{n}_1 \cdot \hat{\mathbf{J}}), (\mathbf{n}_2 \cdot \hat{\mathbf{J}})] + O(\alpha_{1,2}^3).$$

At the same time, to the second order in  $\alpha_{1,2}$  — and hence to the first order in the  $\alpha_3$  — we have

$$\hat{\mathcal{R}}(\mathbf{n}_3, \alpha_3) - 1 = \frac{-i\alpha_3}{\hbar}(\mathbf{n}_3 \cdot \hat{\mathbf{J}}) + O(\alpha_3^2) = \frac{-i\alpha_1\alpha_2}{\hbar}(\mathbf{n}_1 \times \mathbf{n}_2) \cdot \hat{\mathbf{J}} + O(\alpha_{1,2}^4) \quad (87)$$

Consequently, plugging the last two formulae into eq. (82) and focusing on the leading

$O(\alpha_1\alpha_2)$  term, we arrive at

$$-\frac{\alpha_1\alpha_2}{\hbar^2} [(\mathbf{n}_1 \cdot \hat{\mathbf{J}}), (\mathbf{n}_2 \cdot \hat{\mathbf{J}})] = \frac{-i\alpha_1\alpha_2}{\hbar} (\mathbf{n}_1 \times \mathbf{n}_2) \cdot \hat{\mathbf{J}} \quad (88)$$

and hence

$$[(\mathbf{n}_1 \cdot \hat{\mathbf{J}}), (\mathbf{n}_2 \cdot \hat{\mathbf{J}})] = i\hbar(\mathbf{n}_1 \times \mathbf{n}_2) \cdot \hat{\mathbf{J}}. \quad (89)$$

Finally, let's respell eq. (89) in index notations:

$$\begin{aligned} [n_{1i}\hat{J}_i, n_{2j}\hat{J}_j] &= i\hbar\epsilon_{ijk}n_{1i}n_{2j}\hat{J}_k \\ &\parallel \\ n_{1i}n_{2j}[\hat{J}_i, \hat{J}_j] &\quad \langle\langle \text{since } n_{1i} \text{ and } n_{2j} \text{ commute with everything} \rangle\rangle \end{aligned} \quad (90)$$

and since eq. (89) must work for any rotation axes  $\mathbf{n}_1$  and  $\mathbf{n}_2$ , we need

$$[\hat{J}_i, \hat{J}_j] = i\hbar\epsilon_{ijk}\hat{J}_k. \quad (73)$$

Or in vector notations

$$\hat{\mathbf{J}} \times \hat{\mathbf{J}} = i\hbar\hat{\mathbf{J}}. \quad (91)$$

I would like to emphasise that any kind of angular momentum generating 3D rotation of any kind of a quantum system must obey the commutation relations (73). Indeed, we saw back in [homework set#4](#) that the orbital angular momentum  $\hat{\mathbf{L}}$  indeed satisfies the relations (73). Likewise, for a spin =  $\frac{1}{2}$  atom like silver, the spin operator  $\hat{\mathbf{S}} = \frac{\hbar}{2}\vec{\sigma}$  (where  $\sigma_x, \sigma_y, \sigma_z$  are the Pauli matrices) satisfies the same relations:

$$\sigma_i\sigma_j = \delta_{ij}1_{2 \times 2} + i\epsilon_{ijk}\sigma_k \implies [\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k \implies [\hat{S}_i, \hat{S}_j] = i\hbar\epsilon_{ijk}\hat{S}_k. \quad (92)$$

Also, if a system has two kinds of angular momenta acting on different degrees of freedom — such as different particles, or position and spin state of the same particle, — then we should

have

$$[\hat{J}_i^{(1)}, \hat{J}_j^{(1)}] = i\hbar\epsilon_{ijk}\hat{J}_k^{(1)}, \quad [\hat{J}_i^{(2)}, \hat{J}_j^{(2)}] = i\hbar\epsilon_{ijk}\hat{J}_k^{(2)}, \quad \text{but} \quad [\hat{J}_i^{(1)}, \hat{J}_j^{(2)}] = 0. \quad (93)$$

Consequently, the net angular momentum  $\hat{\mathbf{J}}^{\text{net}} = \hat{\mathbf{J}}^{(1)} + \hat{\mathbf{J}}^{(2)}$  automatically obeys the commutation relations (73):

$$\begin{aligned} [\hat{J}_i^{\text{net}}, \hat{J}_j^{\text{net}}] &= [\hat{J}_i^{(1)}, \hat{J}_j^{(1)}] + [\hat{J}_i^{(1)}, \hat{J}_j^{(2)}] + [\hat{J}_i^{(2)}, \hat{J}_j^{(1)}] + [\hat{J}_i^{(2)}, \hat{J}_j^{(2)}] \\ &= i\hbar\epsilon_{ijk}\hat{J}_k^{(1)} + 0 + 0 + i\hbar\epsilon_{ijk}\hat{J}_k^{(2)} \\ &= i\hbar\epsilon_{ijk}\hat{J}_k^{\text{net}}. \end{aligned}$$

Likewise, for the net angular momentum of several degrees of freedom — whatever they are — its components  $(\hat{J}_x^{\text{net}}, \hat{J}_y^{\text{net}}, \hat{J}_z^{\text{net}})$  obey the commutation relations (73).

## Scalars, Vectors, and Tensors

Let's start with the definitions. A vector  $\mathbf{V}$  is more than just an array of three components  $(V_x, V_y, V_z)$ . To make a vector, the three components must transform under a passive rotation of the coordinate system according to

$$V_i \rightarrow V'_i = R_{ij}(\mathbf{n}, \phi)V_j. \quad (94)$$

Likewise, a vector property of a body — or a system of bodies — must transform according to eq. (93) when that body or system is actively rotated in space.

Similarly, a scalar  $S$  is more than a single quantity, it must also be invariant under all passive rotations of the coordinate system. And a scalar property of a body or system stays invariant when that body or system is actively rotated in space.

Many physical quantities are scalars or vectors, but other quantities form *tensors*. For example, the quadrupole moments, the moments of inertia, or the stresses and the strains in some solid body form 2-index tensors  $T_{ij}$ . Again, such a tensor is more than just an array of  $3 \times 3$  components, but these components must transform in a specific manner under

rotations:

$$T'_{ij} = R_{ik}(\mathbf{n}, \alpha)R_{j\ell}(\mathbf{n}, \alpha)T_{j\ell}. \quad (95)$$

Likewise, a 3-index tensor  $T_{ijk}$  is an array of  $3^3$  components which transform under rotations according to

$$T'_{ijk} = R_{i\ell}R_{jm}R_{kn}T_{\ell mn}, \quad (96)$$

and ditto for tensors with more indices.

With these definitions, it is easy to check that for any scalar  $S$  and vectors  $\mathbf{A}$  and  $\mathbf{B}$ :

$$\begin{aligned} S\mathbf{A} & \text{ is a vector,} \\ \mathbf{A} \cdot \mathbf{B} & \text{ is a scalar,} \\ \mathbf{A} \times \mathbf{B} & \text{ is a vector,} \\ T_{ij} = A_i B_j & \text{ is a 2-index tensor.} \end{aligned} \quad (97)$$

Some tensors have symmetry relation between their indices, and the rotations preserve such relations. For example, for a 2-index symmetric tensor

$$T_{ij} = +T_{ji} \implies T'_{ij} = +T'_{ji}, \quad (98)$$

and for a 2-index antisymmetric tensor

$$T_{ij} = -T_{ji} \implies T'_{ij} = -T'_{ji}. \quad (99)$$

Actually, in 3D — and only in 3D — an antisymmetric 2-index tensor is equivalent to a vector,

$$T_{ij} = -T_{ji} = \epsilon_{ijk}V_k, \quad V_k = \frac{1}{2}\epsilon_{kij}T_{ij}, \quad (100)$$

and both of these relations are preserved by the  $SO(3)$  rotations. Also, the trace of a symmetric 2-index tensor  $T_{ij} = +T_{ji}$  is a scalar,

$$\begin{aligned} \text{tr}(T) & \stackrel{\text{def}}{=} T_{ii} = T_{xx} + T_{yy} + T_{zz} \\ & = \text{tr}(T') \quad \text{for any rotation } T' \text{ of } T. \end{aligned} \quad (101)$$

(The proof of both statements a part of problem 2 of [homework set#9](#).)

For the tensors with 3 or more indices, there are many different symmetry patterns. For example:

- totally symmetric tensors,

$$T_{\text{any permutation of } (i,j,\dots,n)} = +T_{(i,j,\dots,n)}; \quad (102)$$

- totally antisymmetric tensors,

$$T_{\text{any permutation of } (i,j,\dots,n)} = T_{(i,j,\dots,n)} \times (-1)^{\text{parity of the permutation}}; \quad (103)$$

- mixed symmetry tensors such as

$$T_{ijk} = +T_{jik} = -T_{ikj} = -T_{kji}. \quad (104)$$

But in 3D, any antisymmetric or mixed-symmetry tensor is equivalent to a totally symmetric tensor with fewer indices. Consequently, any tensor is equivalent to one or several totally symmetric tensors.

#### SCALAR, VECTOR, AND TENSOR OPERATORS

In Quantum Mechanics, we call an operator  $\hat{S}$  a *scalar operator* if and only if all its matrix elements are scalars, *i.e.*, invariant under rotation symmetries:

$$\langle \psi'_1 | \hat{S}' | \psi'_2 \rangle = \langle \psi_1 | \hat{S} | \psi_2 \rangle \quad \text{for any } \langle \psi_1 | \text{ and } | \psi_2 \rangle. \quad (105)$$

In the Schrödinger picture of QM,

$$|\psi'_2\rangle = \hat{\mathcal{R}}(\mathbf{n}, \alpha) |\psi_2\rangle, \quad \langle \psi'_1| = \langle \psi_1| \hat{\mathcal{R}}^\dagger(\mathbf{n}, \alpha), \quad \hat{S}' = \hat{S}, \quad (106)$$

while in the Heisenberg picture

$$|\psi'_2\rangle = |\psi_2\rangle, \quad \langle \psi'_1| = \langle \psi_1|, \quad \hat{S}' = \hat{\mathcal{R}}^\dagger(\mathbf{n}, \alpha) \hat{S} \hat{\mathcal{R}}(\mathbf{n}, \alpha), \quad (107)$$

but in both pictures

$$\langle \psi'_1 | \hat{S}' | \psi'_2 \rangle = \langle \psi_1 | \hat{\mathcal{R}}^\dagger(\mathbf{n}, \alpha) \hat{S} \hat{\mathcal{R}}(\mathbf{n}, \alpha) | \psi_2 \rangle. \quad (108)$$

Plugging this formula into eq. (105), we see that **an operator  $\hat{S}$  is a scalar if and only if**

$$\hat{\mathcal{R}}^\dagger(\mathbf{n}, \alpha) \hat{S} \hat{\mathcal{R}}(\mathbf{n}, \alpha) = \hat{S} \quad (109)$$

for any space rotation  $R(\mathbf{n}, \alpha)$ . Or equivalently,  **$\hat{S}$  is a scalar operator if and only if it commutes with all the rotation operators  $\hat{\mathcal{R}}(\mathbf{n}, \alpha)$ .**

Now consider the vector operators. By definition, we call a trio of component operators  $(\hat{V}_x, \hat{V}_y, \hat{V}_z)$  a *vector operator*  $\hat{\mathbf{V}}$  if and only if the the matrix elements of the components transform into each other under rotations as components of a vector,

$$\langle \psi'_1 | \hat{V}'_i | \psi'_2 \rangle = R_{ij}(\mathbf{n}, \alpha) \langle \psi_1 | \hat{V}_j | \psi_2 \rangle. \quad (110)$$

Similar to the scalar case, the LHS here amounts to

$$\langle \psi_1 | \hat{\mathcal{R}}^\dagger(\mathbf{n}, \alpha) \hat{V}_i \hat{\mathcal{R}}(\mathbf{n}, \alpha) | \psi_2 \rangle, \quad (111)$$

so to make sure eq. (110) holds for the matrix elements between all possible  $\langle \psi_1 |$  and  $| \psi_2 \rangle$ , we need the operatorial identity

$$\hat{\mathcal{R}}^\dagger(\mathbf{n}, \alpha) \hat{V}_i \hat{\mathcal{R}}(\mathbf{n}, \alpha) = R_{ij}(\mathbf{n}, \alpha) \hat{V}_j. \quad (112)$$

In other words,  **$\hat{\mathbf{V}}$  is a vector operator if and only if its components  $\hat{V}_i$  obey eq. (112) for all space rotations.**

Similar rules apply to the tensor operators. For example, 9 component operators  $\hat{T}_{ij}$  form a 2-index tensor operator if and only if their matrix elements transform under rotations as components of a 2-index tensor, or equivalently if and only if for any space rotation

$$\hat{\mathcal{R}}^\dagger(\mathbf{n}, \alpha) \hat{T}_{ij} \hat{\mathcal{R}}(\mathbf{n}, \alpha) = R_{ik}(\mathbf{n}, \alpha) R_{j\ell}(\mathbf{n}, \alpha) \hat{T}_{k\ell}. \quad (113)$$

And ditto for the 3-index tensor operators, *etc.*, *etc.*

All these criteria for the scalar, vector, and tensor operators can be restated in terms of the commutation relations with the angular momentum operators ( $\hat{J}_x, \hat{J}_y, \hat{J}_z$ ) which generate all space rotations,

$$\hat{\mathcal{R}}(\mathbf{n}, \alpha) = \exp((-i\alpha/\hbar)\mathbf{n} \cdot \hat{\mathbf{J}}) \quad (68)$$

Consequently, by the *Baker–Hausdorff lemma*

$$e^{\hat{B}}\hat{C}e^{-\hat{B}} = \hat{C} + [\hat{B}, \hat{C}] + \frac{1}{2}[\hat{B}, [\hat{B}, \hat{C}]] + \cdots + \frac{1}{n!}[\hat{B}, [\hat{B}, \dots, [\hat{B}, \hat{C}] \dots]]_n + \cdots. \quad (114)$$

we may expand the rotated operators of the form

$$\hat{\mathcal{R}}^\dagger(\mathbf{n}, \alpha)\hat{A}\hat{\mathcal{R}}(\mathbf{n}, \alpha) \quad (115)$$

on the left hand sides of eqs. (109), (112), and (113) into multiple commutators of the operator  $\hat{A}$  with  $(\mathbf{n} \cdot \hat{\mathbf{J}})$  and hence with the angular momentum operators ( $\hat{J}_x, \hat{J}_y, \hat{J}_z$ ). Consequently, the criteria (109), (112), and (113) become equivalent to the following commutation relations:

- $\hat{S}$  is a scalar operator if and only if it commutes with the angular momentum,

$$[\hat{S}, \hat{J}_i] = 0. \quad (116)$$

- $\hat{\mathbf{V}}$  is a vector operator if and only if its components obey

$$[\hat{V}_i, \hat{J}_j] = i\hbar\epsilon_{ijk}\hat{V}_k. \quad (117)$$

Note that by this criterion, the angular momentum  $\hat{\mathbf{J}}$  is itself a vector operator.

- $\hat{T}_{ij}$  components comprise a 2-index tensor operator if and only if they obey

$$[\hat{T}_{ij}, \hat{J}_k] = i\hbar\epsilon_{ikl}\hat{T}_{lj} + i\hbar\epsilon_{jkl}\hat{T}_{il}. \quad (118)$$

— Ditto for the tensor operators with 3 or more indices.



Proving that these commutation relations are equivalent to the criteria (109), (112), and (113) is a part of your [homework set#9](#) (problem 2), so I am not going to do it in these notes. Instead, let me simply illustrate these commutation relation in the Hilbert space of a single spinless particle in a central potential. For such a particle  $\hat{\mathbf{J}}$  is simply the orbital angular momentum  $\hat{\mathbf{L}} = \mathbf{x} \times \hat{\mathbf{p}}$ , and we expect  $\hat{\mathbf{x}}$ ,  $\hat{\mathbf{p}}$ , and  $\hat{\mathbf{L}}$  itself to be vector operators, thus

$$[\hat{x}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{x}_k, \quad [\hat{p}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{p}_k, \quad [\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k. \quad (119)$$

On the other hand, we expect the operators  $\hat{r}^2 = \hat{\mathbf{x}}^2$ ,  $\hat{\mathbf{p}}^2$ ,  $\hat{\mathbf{L}}^2$  to be scalar operators, thus

$$[\hat{\mathbf{x}}^2, \hat{L}_j] = 0, \quad [\hat{\mathbf{p}}^2, \hat{L}_j] = 0, \quad [\hat{\mathbf{L}}^2, \hat{L}_j] = 0. \quad (120)$$

And indeed, back in [homework set#4](#) (problem 2) we saw that all these commutation relation hold true.

## Lie Groups and Lie Algebras

Let's go back to general symmetries, or rather to the general *continuous* symmetries. Mathematically, such symmetries form a *Lie groups* — a group whose elements  $S$  also form a differentiable manifold of some dimension  $N$ . In other words, we may continuously — and differentiably — parametrize the symmetries by  $N$  independent real variables,  $(a_1, \dots, a_N)$ , and we may always chose such parameters such that  $S(0, \dots, 0) = 1$  while for the infinitesimal  $(da_1, \dots, da_N)$  the symmetry  $S(da_1, \dots, da_N)$  is infinitesimally close to the identity. For example, the 3D rotations  $R(\mathbf{n}, \alpha)$  can be re-parametrized as  $R(a_x, a_y, a_z)$  for  $(a_x, a_y, a_z) = (\alpha n_x, \alpha n_y, \alpha n_z)$ .

In quantum mechanics, such symmetries are represented by unitary operators

$$\begin{aligned} \hat{U}(a_1, \dots, a_N) &= \hat{U}(S(a_1, \dots, a_N)) \\ \text{which is a differentiable function of the } (a_1, \dots, a_N), & \quad (121) \\ \hat{U}(0, \dots, 0) &= 1. \end{aligned}$$

So let's define  $N$  *generators of the symmetry group* as the derivatives

$$\hat{\mathcal{T}}_i \stackrel{\text{def}}{=} i\hbar \left. \frac{\partial \hat{U}}{\partial a_i} \right|_{a_1=\dots=a_N=0}, \quad i = 1, \dots, N. \quad (122)$$

By unitarity of the symmetry operators  $\hat{U}(a_1, \dots, a_n)$ , these generators are Hermitian oper-

ators. Indeed, to the first order in the the infinitesimal parameters  $da_i$ ,

$$\hat{U}(da_1, \dots, da_N) = 1 - \frac{i}{\hbar} \sum_{i=1}^N \hat{\mathcal{T}}_i da_i + O(da^2), \quad (123)$$

hence

$$\hat{U}^\dagger(da_1, \dots, da_N) = 1 + \frac{i}{\hbar} \sum_{i=1}^N \hat{\mathcal{T}}_i^\dagger da_i + O(da^2), \quad (124)$$

and

$$U^\dagger U = 1 - \frac{i}{\hbar} \sum_{i=1}^N (\hat{\mathcal{T}}_i - \hat{\mathcal{T}}_i^\dagger) da_i + O(da^2). \quad (125)$$

But the symmetry operator  $\hat{U}(da_1, \dots, da_n)$  must be unitary,  $\hat{U}^\dagger \hat{U} = 1$ , so the  $O(da)$  term on the RHS here must vanish for any infinitesimal  $(da_1, \dots, da_n)$ , thus  $\hat{\mathcal{T}}_i - \hat{\mathcal{T}}_i^\dagger = 0$ . In other words, all  $N$  generators  $\hat{\mathcal{T}}_i$  must be Hermitian operators.

To see how the operators  $\hat{\mathcal{T}}_i$  generate the finite symmetry transformations  $\hat{U}(a_1, \dots, a_N)$ , let us choose the parameters  $(a_1, \dots, a_N)$  of the finite symmetries such that

$$S(a_1, \dots, a_N) = \left[ S\left(\frac{a_1}{m}, \dots, \frac{a_N}{m}\right) \right]^m, \quad (126)$$

similarly to what we have for the rotations parametrized by the  $\mathbf{a} = \alpha \mathbf{n}$ :  $R(\alpha n_x, \alpha n_y, \alpha n_z) = \left[ R\left(\frac{\alpha n_x}{m}, \frac{\alpha n_y}{m}, \frac{\alpha n_z}{m}\right) \right]^m$ . Then,

$$\begin{aligned} \hat{U}(a_1, \dots, a_N) &= \left[ \hat{U}\left(\frac{a_1}{m}, \dots, \frac{a_N}{m}\right) \right]^m \\ &\quad \langle\langle \text{where all } \frac{a_i}{m} \text{ become infinitesimal for } m \rightarrow \infty \rangle\rangle \\ &= \lim_{m \rightarrow \infty} \left[ 1 - \frac{i}{\hbar} \sum_i \frac{a_i}{m} \hat{\mathcal{T}}_i + O(a^2/m^2) \right]^m \\ &= \lim_{m \rightarrow \infty} \left[ 1 + \frac{1}{m} \left( \frac{-i}{\hbar} \sum_i a_i \hat{\mathcal{T}}_i \right) + O(1/m^2) \right]^m \\ &= \exp\left(\frac{-i}{\hbar} \sum_i a_i \hat{\mathcal{T}}_i\right). \end{aligned} \quad (127)$$

For example, the 3D rotation symmetries are generated by the angular momentum  $\hat{\mathbf{J}}$ ,

$$\hat{J}_i = i\hbar \left. \frac{\partial \hat{\mathcal{R}}(\alpha \mathbf{n})}{\partial (\alpha \mathbf{n})_i} \right|_{\alpha \mathbf{n}=0}, \quad \hat{\mathcal{R}}(\text{finite } \alpha \mathbf{n}) = \exp\left(\frac{-i}{\hbar} \alpha \mathbf{n} \cdot \hat{\mathbf{J}}\right), \quad (128)$$

while the space translation symmetries are generated by the linear momentum  $\hat{\mathbf{P}}$ ,

$$\hat{P}_i = i\hbar \left. \frac{\partial \hat{T}(\mathbf{a})}{\partial a_i} \right|_{\mathbf{a}=0}, \quad \hat{T}(\text{finite } \mathbf{a}) = \exp\left(\frac{-i}{\hbar} \mathbf{a} \cdot \hat{\mathbf{P}}\right). \quad (129)$$

Clearly, the generators of an abelian symmetry group — like the translations — must commute with each other,  $[\hat{\mathcal{T}}_i, \hat{\mathcal{T}}_j] = 0$ , while the generators of a non-abelian group — like the 3D rotations — should not commute. Instead, **the commutators of the non-abelian group's generators are linear combinations of the other generators**,

$$[\hat{\mathcal{T}}_i, \hat{\mathcal{T}}_j] = i\hbar \sum_k f_{ijk} \hat{\mathcal{T}}_k \quad (130)$$

for some constant coefficients  $f_{ijk}$ , called *the structure constants* of the symmetry group in question. Similarly to what we did for the  $SO(3)$  rotation symmetry — for which  $f_{ijk} = \epsilon_{ijk}$ , thus  $[\hat{J}_i, \hat{J}_j] = i\hbar \epsilon_{ijk} \hat{J}_k$ , — the structure constants for other non-abelian symmetries obtain by looking at the infinitesimal symmetries  $S(da_1, \dots, da_N)$  and their products to the second order in  $da_i$ . In general, all infinitesimal symmetries commute to first order in  $da$ ,

$$S(db_1, \dots, db_n) \times S(da_1, \dots, da_N) = S(da_1, \dots, da_N) \times S(db_1, \dots, db_n) + O(da \times db), \quad (131)$$

while to the second order in  $da$  and  $db$  we have

$$S(db_1, \dots, db_n) \times S(da_1, \dots, da_N) = S(da_1, \dots, da_N) \times S(db_1, \dots, db_n) \times S(dc_1, \dots, dc_N) \quad (132)$$

for some

$$dc_k = \sum_{ijk} da_i db_j f_{ijk} + O(da^2 db \text{ or } da db^2). \quad (133)$$

For example, eqs. (80) and (81) for the rotation symmetries become in present notations

$$R(d\mathbf{b}) \times R(d\mathbf{a}) = R(d\mathbf{a}) \times R(d\mathbf{b}) \times R(d\mathbf{c}) \quad (134)$$

for

$$d\mathbf{c} = d\mathbf{a} \times d\mathbf{b} + O(da^2 db \text{ or } da db^2), \quad (135)$$

which corresponds to  $f_{ijk} = \epsilon_{ijk}$ .

For other symmetry groups we would have some other structure constants  $f_{ijk}$  and hence different commutation algebras — AKA Lie algebras — (130). Indeed, eq. (132) for the symmetries themselves translates to

$$\hat{U}(db_1, \dots, db_n) \times \hat{U}(da_1, \dots, da_N) = \hat{U}(da_1, \dots, da_N) \times \hat{U}(db_1, \dots, db_n) \times \hat{U}(dc_1, \dots, dc_N), \quad (136)$$

hence to the second order in  $da$  and  $db$  and the first order in  $dc$ ,

$$\frac{-1}{\hbar^2} \sum_{ij} da_i db_j \hat{\mathcal{T}}_i \hat{\mathcal{T}}_j = \frac{-1}{\hbar^2} \sum_{ij} db_j da_i \hat{\mathcal{T}}_j \hat{\mathcal{T}}_i - \frac{i}{\hbar} \sum_k dc_k \hat{\mathcal{T}}_k + \text{higher orders} \quad (137)$$

and therefore

$$\sum_{ij} da_i db_j [\hat{\mathcal{T}}_i, \hat{\mathcal{T}}_j] = i\hbar \sum_k dc_k \hat{\mathcal{T}}_k + \text{higher orders}. \quad (138)$$

Since the  $dc_k$  in this formula should be exactly as in eq. (133), this means

$$\sum_{ij} da_i db_j [\hat{\mathcal{T}}_i, \hat{\mathcal{T}}_j] = i\hbar \sum_{ijk} da_i db_j f_{ijk} \hat{\mathcal{T}}_k \quad (139)$$

and therefore

$$[\hat{\mathcal{T}}_i, \hat{\mathcal{T}}_j] = i\hbar \sum_k f_{ijk} \hat{\mathcal{T}}_k. \quad (140)$$

Thus, we see that the non-abelian group product of the infinitesimal symmetries completely determines the commutator algebra of the group's generators. Conversely, the commutator algebra of the generators completely determines the products of all the finite symmetries. Indeed, consider the [Baker–Campbell–Hausdorff formula](#): for any matrices or operators  $\hat{X}$  and  $\hat{Y}$ ,

$$\exp(\hat{X}) \exp(\hat{Y}) = \exp(\hat{Z}) \quad (140)$$

where  $\hat{Z}$  is a series in multiple commutators of  $\hat{X}$  and  $\hat{Y}$ ,

$$\hat{Z} = \hat{X} + \hat{Y} + \frac{1}{2}[\hat{X}, \hat{Y}] + \frac{1}{12}[(\hat{X} - \hat{Y}), [\hat{X}, \hat{Y}]] - \frac{1}{24}[\hat{Y}, [\hat{X}, [\hat{X}, \hat{Y}]]] + \dots \quad (141)$$

Note that the product of any two finite symmetries

$$\hat{U}(a_1, \dots, a_n) \times \hat{U}(b_1, \dots, b_n) = \exp\left(\frac{-i}{\hbar} \sum_i a_i \hat{\mathcal{T}}_i\right) \times \exp\left(\frac{-i}{\hbar} \sum_j b_j \hat{\mathcal{T}}_j\right) \quad (142)$$

has the form of the BCH formula's LHS for

$$\hat{X} = \frac{-i}{\hbar} \sum_i a_i \hat{\mathcal{T}}_i, \quad \hat{Y} = \frac{-i}{\hbar} \sum_j b_j \hat{\mathcal{T}}_j. \quad (143)$$

As to the RHS of that formula, all multiple commutators of these  $\hat{X}$  and  $\hat{Y}$  obtain from the Lie algebra (130):

$$[\hat{X}, \hat{Y}] = \frac{-i}{\hbar} \sum_{i,j,k} a_i b_j f_{ijk} \hat{\mathcal{T}}_k, \quad (144)$$

$$[(\hat{X} - \hat{Y}), [\hat{X}, \hat{Y}]] = \frac{-i}{\hbar} \sum_{i,j,k,\ell,m} (a_i - b_i) a_j b_k f_{jkl} f_{ilm} \hat{\mathcal{T}}_m, \quad (145)$$

*etc., etc.*

Altogether, on the RHS of the BCH formula we end up with

$$\hat{Z} = \frac{-i}{\hbar} \sum_m c_m \hat{\mathcal{T}}_m \quad (146)$$

where the coefficients  $c_m$  are power series in the  $a_i$  and  $b_j$ ,

$$c_m = a_m + b_m + \frac{1}{2} \sum_{i,j} a_i b_j f_{ijm} + \frac{1}{12} \sum_{i,j,k,\ell} (a_i - b_i) a_j b_k f_{jkl} f_{ilm} + \dots, \quad (147)$$

and therefore

$$\hat{U}(a_1, \dots, a_n) \times \hat{U}(b_1, \dots, b_n) = \hat{U}(c_1, \dots, c_m) \quad (148)$$

where the parameters  $(c_1, \dots, c_N)$  of the product obtain as the power series (147) in the parameters  $(a_1, \dots, a_n)$  and  $(b_1, \dots, b_n)$  of the two factors.

## Representations and Multiplets

A *representation* of a group  $G$  is a map from  $G$  to the space of matrices or operators,  $S \mapsto M(S)$  or  $S \mapsto \hat{U}(S)$  such that

$$\begin{aligned} M(\text{group product } S_2 S_1) &= \text{matrix product } M(S_2)M(S_1) \\ \text{or } \hat{U}(\text{group product } S_2 S_1) &= \text{operator product } \hat{U}(S_2)\hat{U}(S_1). \end{aligned} \tag{149}$$

A point of terminology: a representation by finite  $n \times n$  matrices is called a finite representation of dimension  $n$ , while a representation by operators in an infinite-dimensional Hilbert space is called an infinite representation.

The same group  $G$  may have an infinite variety of different representations. For example, for any rotationally symmetric quantum system, the unitary rotation operators  $\hat{\mathcal{R}}(\mathbf{n}, \alpha)$  form a representation of the rotation group. Moreover, the same rotation group has an infinite series of finite representations of dimensions  $n = 1, 2, 3, 4, \dots$ . For example, the  $SO(3)$  matrices

$$R_{ij}(\mathbf{n}, \alpha) = \cos \alpha \delta_{ij} + \sin \alpha n_k \epsilon_{ikj} + (1 - \cos \alpha) n_i n_j \tag{58}$$

form a 3-dimensional representation of the rotation group, while the  $SU(2)$  matrices

$$U_{\alpha\beta}(\mathbf{n}, \alpha) = \left( \exp\left(-i\frac{\alpha}{2} \mathbf{n} \cdot \vec{\sigma}\right) \right)_{\alpha\beta} = \cos \frac{\alpha}{2} \delta_{\alpha\beta} - i \sin \frac{\alpha}{2} n_k (\sigma_k)_{\alpha\beta} \tag{150}$$

(where  $\sigma_{x,y,z}$  are Pauli matrices) form a 2-dimensional representation. (The proof is a part of the [homework set#9](#), problem 1.)

A representation is called *reducible* if all the matrices  $M(S)$  or operators  $\hat{U}(S)$  are block-diagonal in the same basis. In this case, every diagonal block by itself is a smaller representation of the same symmetry group. A representation by matrices which cannot be block-diagonalized in the same basis is called *irreducible*. By these definitions, a reducible representation is a tensor sum of its irreducible diagonal blocks,

$$(r)_{\text{net}} = (r)_1 \oplus (r)_2 \oplus \dots, \tag{151}$$

so once we classify all the irreducible representations of some group  $G$ , all the reducible representations obtain as tensor sums (151).

Now consider a Lie algebra (the commutator algebra) of some continuous symmetry group. A representation ( $r$ ) of the Lie algebra is a set of finite matrices  $T_i^{(r)}$  or operators  $\hat{T}_i^{(r)}$  which obey the same commutation relations as the algebra's generators  $\hat{T}_i$ ,

$$[T_i^{(r)}, T_j^{(r)}] = i\hbar \sum_k f_{ijk} T_k^{(r)}. \quad (152)$$

Any representation of a Lie algebra can be turned into a representation of the corresponding Lie group by matrix exponentiation: for  $S(a_1, \dots, a_N)$  such that

$$\hat{U}(S(a_1, \dots, a_N)) = \text{operator exp} \left( \frac{-i}{\hbar} \sum_i a_i \hat{T}_i \right), \quad (153)$$

we let

$$M^{(r)}(a_1, \dots, a_N) = \text{matrix exp} \left( \frac{-i}{\hbar} \sum_i a_i T_i^{(r)} \right). \quad (154)$$

Then by the Baker–Campbell–Hausdorff formula, for

$$S(c_1, \dots, c_N) = S(a_1, \dots, a_N) \times S(b_1, \dots, b_N) \quad (155)$$

we get

$$M^{(r)}(c_1, \dots, c_N) = M^{(r)}(a_1, \dots, a_N) \times M^{(r)}(b_1, \dots, b_N) \quad (156)$$

in the same way as

$$\hat{U}(c_1, \dots, c_N) = \hat{U}(a_1, \dots, a_N) \times \hat{U}(b_1, \dots, b_N). \quad (157)$$

For example, a representation ( $r$ ) of the angular momentum algebra is a set of 3 matrices  $J_x^{(r)}$ ,  $J_y^{(r)}$ , and  $J_z^{(r)}$  such that

$$[J_i^{(r)}, J_j^{(r)}] = i\hbar \epsilon_{ijk} J_k^{(r)}, \quad (158)$$

and any such representation can be turned into a representation of the rotation group as

$$M^{(r)}(\mathbf{n}, \alpha) = \text{matrix exp} \left( \frac{-i}{\hbar} \alpha \mathbf{n} \cdot \mathbf{J}^{(r)} \right). \quad (159)$$

In particular, the  $2 \times 2$  Hermitian matrices  $J_i^{(2)} = \frac{1}{2}\hbar\sigma_i$ ,

$$J_x^{(2)} = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad J_y^{(2)} = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}, \quad J_z^{(2)} = \frac{\hbar}{2} \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix} \quad (160)$$

generate the 2-dimensional representation (150) of the rotation group, while the  $3 \times 3$  imaginary antisymmetric (and hence Hermitian) matrices

$$(J_i^{(3)})_{jk} = i\hbar\epsilon_{jik}, \quad (161)$$

— or in explicit matrix form

$$J_x^{(3)} = \hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & +i & 0 \end{pmatrix}, \quad J_y^{(3)} = \hbar \begin{pmatrix} 0 & 0 & +i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad J_z^{(3)} = \hbar \begin{pmatrix} 0 & -i & 0 \\ +i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (162)$$

— generate the 3-dimensional representation by the  $SO(3)$  rotation matrices (58) themselves.

Now consider symmetries of a quantum system. The unitary operators  $\hat{U}(S)$  in the Hilbert space of the system form an infinite representation of the symmetry group  $G$ . But usually, this representation is highly reducible, so in some basis  $\{|\alpha, \mu\rangle\}$  the matrix elements of all the symmetries become block-diagonal,

$$\langle \alpha, \mu | \hat{U}(S) | \beta, \nu \rangle = \delta_{\alpha, \beta} \times U_{\mu, \nu}^{(\alpha)}(S), \quad (163)$$

for some matrices  $U_{\mu, \nu}^{(\alpha)}(S)$ . The states  $|\alpha, \mu\rangle$  belonging to the same block  $\alpha$  form a *multiplet* of the symmetry group: Under the symmetry transforms, the states in a multiplet mix with each other but not with any states in other multiplets,

$$\hat{U}(S) |\alpha, \nu\rangle = \sum_{\mu} |\alpha, \mu\rangle \times U_{\mu, \nu}^{(\alpha)}(S) \quad \text{but no terms with } \beta \neq \alpha. \quad (164)$$

The multiplets of a symmetry is closely related to the representations as all the matrices  $U_{\mu, \nu}^{(\alpha)}(S)$  form representations of the symmetry group, thus

$$U_{\mu, \nu}^{(\alpha)}(S) = M_{\mu, \nu}^{(r)}(S) \quad \text{for some representation } (r). \quad (165)$$

However, the representations  $(r)$  are classified just by the matrices  $M_{\mu, \nu}^{(r)}(S)$  regardless of which states are transformed according to this matrix, so different multiplets  $\alpha \neq \beta$  may



transform according to the same representation of the symmetry. In other words, *the representation is the multiplet type*, but the Hilbert space may contain many distinct multiplets of the same type.

For example, consider the rotational symmetry of a spinless particle in a central potential. As you (should have) learned in the undergraduate school, the Hamiltonian eigenstates for such a particle are labeled by the radial quantum number  $n_r$ , the orbital quantum number  $\ell$ , and the magnetic quantum number  $m$ ; they have wave-functions of the form

$$\Psi_{n_r, \ell, m}(r, \theta, \phi) = \psi_{n_r, \ell}(r) \times Y_{\ell, m}(\theta, \phi) \quad (166)$$

and energies  $E(n_r, \ell)$  which are degenerate WRT  $m$ ,

$$\hat{H} |n_r, \ell, m\rangle = E(n_r, \ell \text{ only}) |n_r, \ell, m\rangle. \quad (167)$$

As we shall see in a few pages, the rotational symmetries act in this basis as

$$\hat{\mathcal{R}}(\mathbf{n}, \alpha) |n_r, \ell, m\rangle = \sum_{m' \text{ only}} |n_r, \ell, m'\rangle \times \mathcal{D}_{m', m}^{(\ell)}(\mathbf{n}, \alpha). \quad (168)$$

Thus, states with the same  $n_r$  and  $\ell$  but different  $m$  form a multiplet — the rotations do not mix them up with the other states. In other words, the quantum numbers  $n_r$  and  $\ell$  label multiplets while  $m$  labels states within the multiplets. Furthermore, the transformation matrices  $\mathcal{D}_{m, m'}^{(\ell)}(\mathbf{n}, \alpha)$  for the members of a multiplet  $(n_r, \ell)$  depend on  $\ell$  but not on the  $n_r$ . Thus, we have the same representation ( $\ell$ ) of the rotation group for all multiplets  $(n_r, \ell)$  with the same  $\ell$  but different  $n_r$ .

I shall return to this issue once we have classified the representations of the angular momentum algebra and hence of the rotation group.

## Representations of the Angular Momentum

To classify the (finite, unitary, and irreducible) representation of the angular momentum algebra, consider a generic quantum system with a rotational symmetry and its generators  $\hat{J}_{x,y,z}$ . The key to our classification is the operator  $\hat{\mathbf{J}}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$  and its spectrum. The most important feature of the  $\hat{\mathbf{J}}^2$  operator is that it commutes with all 3 generators  $\hat{J}_{x,y,z}$ :

$$\begin{aligned} [\hat{J}_i, \hat{\mathbf{J}}^2] &= [\hat{J}_i, \hat{J}_j \hat{J}_j] = [\hat{J}_i, \hat{J}_j] \hat{J}_j + \hat{J}_j [\hat{J}_i, \hat{J}_j] \\ &= (i\hbar \epsilon_{ijk} \hat{J}_k) \hat{J}_j + \hat{J}_j (i\hbar \epsilon_{ijk} \hat{J}_k) = i\hbar \epsilon_{ijk} \{ \hat{J}_j, \hat{J}_k \} \\ &= 0 \quad \text{because } \epsilon_{ijk} = -\epsilon_{ikj} \text{ while } \{ \hat{J}_j, \hat{J}_k \} = +\{ \hat{J}_k, \hat{J}_j \}. \end{aligned} \tag{169}$$

The  $\hat{\mathbf{J}}^2$  is the *quadratic Casimir operator* of the angular momentum algebra. Other Lie algebras also have quadratic Casimir operators of the form

$$\hat{C}_2 = \sum_{ij} g_{ij} \hat{T}_i \hat{T}_j \tag{170}$$

where the metric  $g_{ij}$  is chosen such that the  $\hat{C}_2$  commutes with all the generators,  $[\hat{C}_2, \hat{T}_i] = 0$ .

Since the angular momentum operators  $\hat{J}_{x,y,z}$  do not commute, we cannot diagonalize all of them in the same basis; but we can simultaneously diagonalize the  $\hat{\mathbf{J}}^2$  operator and one of the generators, say the  $\hat{J}_z$ . Since  $\hat{\mathbf{J}}^2$  is a non-negative Hermitian operator, its eigenvalues are non-negative real numbers; for future convenience, we shall write them as

$$\text{eigenvalue}(\hat{\mathbf{J}}^2) = \hbar^2 j(j+1) \quad \text{for } j \geq 0. \tag{171}$$

Likewise, we shall write the eigenvalues of  $\hat{J}_z$  as  $\hbar m$ , but  $m$  may be positive or negative (or zero). Altogether, we look for a basis of the states  $|\alpha, j, m\rangle$  where

$$\begin{aligned} \hat{\mathbf{J}}^2 |\alpha, j, m\rangle &= \hbar^2 j(j+1) |\alpha, j, m\rangle, \\ \hat{J}_z |\alpha, j, m\rangle &= \hbar m |\alpha, j, m\rangle, \end{aligned} \tag{172}$$

and  $\alpha$  distinguishes different states with the same  $j$  and  $m$ .

A while ago, we have seen how for a Harmonic oscillator, the commutation relation  $[\hat{a}, \hat{a}^\dagger] = 1$  completely determines the spectrum of the operator  $\hat{n} = \hat{a}^\dagger \hat{a}$  and hence of

the oscillator's Hamiltonian. For the angular momentum, we have a similar situation: the Hermiticity of the generators  $\hat{J}_i^\dagger = \hat{J}_i$  and their commutation relations  $[\hat{J}_i, \hat{J}_j] = i\hbar\epsilon_{ijk}\hat{J}_k$  completely determine the mutual spectrum of the operators  $\hat{\mathbf{J}}^2$  and  $\hat{J}_z$ .

For the harmonic oscillator, we have raising/lowering operators  $\hat{a}^\dagger$  and  $\hat{a}$  which raise/lower  $n$  by  $\pm 1$ . For the angular momentum, we have similar raising/lowering operators

$$\hat{J}_\pm \stackrel{\text{def}}{=} \hat{J}_x \pm i\hat{J}_y, \quad (\hat{J}_\pm)^\dagger = \hat{J}_\mp \quad (173)$$

which raise/lower  $m$  by  $\pm 1$  while leaving  $j$  unchanged. Indeed,

$$[\hat{\mathbf{J}}^2, \hat{J}_\pm] = [\hat{\mathbf{J}}^2, \hat{J}_x] \pm i[\hat{\mathbf{J}}^2, \hat{J}_y] = 0 \pm i0 = 0, \quad (174)$$

while

$$\begin{aligned} [\hat{J}_z, \hat{J}_\pm] &= [\hat{J}_z, \hat{J}_x] \pm i[\hat{J}_z, \hat{J}_y] \\ &= i\hbar\hat{J}_y \pm i(-i\hbar\hat{J}_x) = \pm\hbar(\hat{J}_x \pm i\hat{J}_y) \\ &= \pm\hbar\hat{J}_\pm, \end{aligned} \quad (175)$$

or in other words

$$\hat{J}_z\hat{J}_\pm = \hat{J}_\pm(\hat{J}_z \pm \hbar). \quad (176)$$

Now let  $|\Psi\rangle = \hat{J}_\pm|\alpha, j, m\rangle$  and assume  $|\Psi\rangle \neq 0$ . Then  $|\Psi\rangle$  is a state of definite  $j' = j$  and definite  $m' = m \pm 1$ . Indeed,

$$\begin{aligned} \hat{\mathbf{J}}^2|\Psi\rangle &= \hat{\mathbf{J}}^2\hat{J}_\pm|\alpha, j, m\rangle = \hat{J}_\pm\hat{\mathbf{J}}^2|\alpha, j, m\rangle = \hat{J}_\pm(\hbar^2j(j+1)|\alpha, j, m\rangle) \\ &= \hbar^2j(j+1)\hat{J}_\pm|\alpha, j, m\rangle = \hbar^2j(j+1)|\Psi\rangle, \end{aligned} \quad (177)$$

while

$$\begin{aligned} \hat{J}_z|\Psi\rangle &= \hat{J}_z\hat{J}_\pm|\alpha, j, m\rangle = \hat{J}_\pm(\hat{J}_z \pm \hbar)|\alpha, j, m\rangle \\ &= \hat{J}_\pm(\hbar m|\alpha, j, m\rangle \pm \hbar|\alpha, j, m\rangle) = \hbar(m \pm 1)\hat{J}_\pm|\alpha, j, m\rangle \\ &= \hbar(m \pm 1)|\Psi\rangle. \end{aligned} \quad (178)$$

Thus,  $|\Psi\rangle$  must be a linear combination of states  $|\alpha', j, m \pm 1\rangle$ .

Next, consider the operator product

$$\begin{aligned}\hat{J}_\mp \hat{J}_\pm &= (\hat{J}_x \mp i\hat{J}_y)(\hat{J}_x \pm i\hat{J}_y) = \hat{J}_x^2 + \hat{J}_y^2 \pm i[\hat{J}_x, \hat{J}_y] \\ &= \hat{\mathbf{J}}^2 - \hat{J}_z^2 \mp \hbar\hat{J}_z.\end{aligned}\tag{179}$$

Acting with this operator product on the state  $|\alpha, j, m\rangle$ , we get the state

$$\begin{aligned}\hat{J}_\mp \hat{J}_\pm |\alpha, j, m\rangle &= \hat{\mathbf{J}}^2 |\alpha, j, m\rangle - \hat{J}_z^2 |\alpha, j, m\rangle \mp \hbar\hat{J}_z |\alpha, j, m\rangle \\ &= \hbar^2 j(j+1) |\alpha, j, m\rangle - \hbar^2 m^2 |\alpha, j, m\rangle \mp \hbar^2 m |\alpha, j, m\rangle \\ &= \hbar^2 (j(j+1) - m^2 \mp m) |\alpha, j, m\rangle\end{aligned}\tag{180}$$

with exactly the same  $\alpha$ ,  $j$ , and  $m$ . Thus, when we use operators  $\hat{J}_+$  and  $\hat{J}_-$  to move between the states  $|\alpha, j, m\rangle$  and  $|\alpha', j, m+1\rangle$ ,

$$|\alpha, j, m\rangle \begin{array}{c} \xrightarrow{\hat{J}_+} \\ \xleftarrow{\hat{J}_-} \end{array} |\alpha', j, m+1\rangle,\tag{181}$$

going both ways brings us back to exactly the same state we have started from. Consequently, we may reorganize the basis of  $\alpha'$  for the states  $|\alpha', j, m+1\rangle$  so that we have the same  $\alpha$  on both sides of this diagram, thus

$$|\alpha, j, m\rangle \begin{array}{c} \xrightarrow{\hat{J}_+} \\ \xleftarrow{\hat{J}_-} \end{array} |\alpha, j, m+1\rangle,\tag{182}$$

Likewise, we may rearrange the basis of  $\alpha'$  for the states  $|\alpha', j, m-1\rangle$  so that

$$|\alpha, j, m-1\rangle \begin{array}{c} \xrightarrow{\hat{J}_+} \\ \xleftarrow{\hat{J}_-} \end{array} |\alpha, j, m\rangle,\tag{183}$$

works for the same  $\alpha$  on both sides of the diagram. Naturally, we can repeat this procedure for all the other  $|\alpha, j, m'\rangle$  states using several raising/lowering operators  $\hat{J}_+$  and  $\hat{J}_-$ , which

gets us a whole chain of states with the same  $\alpha$  and  $j$  but different  $m$ :

$$\cdots \begin{array}{c} \hat{J}_+ \\ \longleftrightarrow \\ \hat{J}_- \end{array} |\alpha, j, m-2\rangle \begin{array}{c} \hat{J}_+ \\ \longleftrightarrow \\ \hat{J}_- \end{array} |\alpha, j, m-1\rangle \begin{array}{c} \hat{J}_+ \\ \longleftrightarrow \\ \hat{J}_- \end{array} |\alpha, j, m+0\rangle \begin{array}{c} \hat{J}_+ \\ \longleftrightarrow \\ \hat{J}_- \end{array} |\alpha, j, m+1\rangle \begin{array}{c} \hat{J}_+ \\ \longleftrightarrow \\ \hat{J}_- \end{array} |\alpha, j, m+2\rangle \begin{array}{c} \hat{J}_+ \\ \longleftrightarrow \\ \hat{J}_- \end{array} \cdots \quad (184)$$

Each step here changes  $m$  by  $\pm 1$ .

For the harmonic oscillator we had similar chains of  $|\alpha, n\rangle$  states, and all such chains terminated at the lower end  $n_{\min} = 0$  but run to  $n \rightarrow +\infty$  at the upper end. By contrast, the chain (184) of the angular momentum states must terminate at both ends. To see that, consider the operators  $\hat{J}_\mp \hat{J}_\pm$ : Since  $\hat{J}_+$  and  $\hat{J}_-$  are Hermitian conjugates of each other, both  $\hat{J}_+ \hat{J}_-$  and  $\hat{J}_- \hat{J}_+$  are Hermitian non-negative operators, so all their eigenvalues must be real and non-negative. At the same time, we have

$$\hat{J}_\mp \hat{J}_\pm |\alpha, j, m\rangle = \hbar^2 (j(j+1) - m^2 \mp m) |\alpha, j, m\rangle, \quad (180)$$

which means that for any  $|\alpha, j, m\rangle$  state we must have

$$j(j+1) - m^2 \mp m \geq 0 \quad . \quad (185)$$

Combining these equations for both signs of  $\mp$ , we get

$$j(j+1) \geq |m|^2 + |m| \quad (186)$$

and hence

$$-j \leq m \leq +j. \quad (187)$$

And that's why the chain (184) must terminate at both ends.

Now consider the top of the chain, the state  $|\alpha, j, m_{\max}\rangle$  with the highest  $m = m_{\max}$ . To keep the chain from extending to still higher  $m > m_{\max}$ , we need  $\hat{J}_+ |\alpha, j, m_{\max}\rangle = 0$  and

hence  $\hat{J}_- \hat{J}_+ |\alpha, j, m_{\max}\rangle = 0$ . In light of eq. (180), this calls for

$$j(j+1) - m_{\max}^2 - m_{\max} = 0, \quad (188)$$

and this quadratic equation has 2 solutions:  $m_{\max} = +j$  or  $m_{\max} = -j - 1$ . However, only the first solution satisfies the limit (187), thus

$$m_{\max} = +j. \quad (189)$$

Similarly, at the bottom of the chain (184) we have the state  $|\alpha, j, m_{\min}\rangle$  with the lowest  $m = m_{\min}$ . To keep the chain from running to the still lower  $m < m_{\min}$  we need  $\hat{J}_- |\alpha, j, m_{\min}\rangle = 0$  and hence  $\hat{J}_+ \hat{J}_- |\alpha, j, m_{\min}\rangle = 0$ . Again, in light of eq. (180), this requirement calls for

$$j(j+1) - m_{\min}^2 + m_{\min} = 0 \quad (190)$$

and hence either  $m_{\min} = +j + 1$  or  $m_{\min} = -j$ . But this time, only the second solution satisfies the limit (187), thus

$$m_{\min} = -j. \quad (191)$$

Altogether, we have  $m$  running from  $-j$  to  $+j$  by 1,

$$m = (-j), (1-j), \dots, (j-1), (+j). \quad (192)$$

Consequently,  $2j$  must be an integer! Thus,

$$\begin{aligned} &\text{either } j \text{ is a non-negative integer, } j = 0, 1, 2, 3, \dots, \\ &\text{or } j \text{ is a positive half-integer, } j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots \end{aligned} \quad (193)$$

Furthermore, for an integer  $j$ ,  $m$  should also be integer, while for a half-integer  $j$ ,  $m$  should also be half-integer. For example, for  $j = \frac{1}{2}$ ,  $m$  takes values  $-\frac{1}{2}$  and  $+\frac{1}{2}$  but not 0.

Note that we derived these quantization rules without any assumptions about the nature of the quantum system in question besides having a 3D rotational symmetry. The system may involve spins and other degrees of freedom unrelated to the particle's motion that contribute to the net angular momentum  $\hat{\mathbf{J}}$ . But for all such systems, the very structure of the  $SO(3)$  rotation group guarantees that the angular momenta have quantized eigenvalues:  $j(j+1)\hbar^2$  for the  $\hat{\mathbf{J}}^2$  and  $m\hbar$  for the  $\hat{J}_z$ , with integer or half-integer  $j$  and  $m$ .

#### MATRIX ELEMENTS, MULTIPLICETS, AND REPRESENTATIONS.

The chain (184) of states  $|\alpha, j, m\rangle$  for fixed  $\alpha$  and  $j$ , and all  $m$  running from  $-j$  to  $+j$  by 1 comprises a multiplet of the angular momentum algebra. Indeed,

$$\left. \begin{aligned} \hat{J}_z |\alpha, j, m\rangle &= \hbar m |\alpha, j, m\rangle, \\ \hat{J}_\pm |\alpha, j, m\rangle &= \text{coefficient} \times |\alpha, j, m \pm 1\rangle, \end{aligned} \right\} \text{ for the same } \alpha \text{ and } j. \quad (194)$$

As to the coefficients on the second line here, their magnitudes obtain from

$$\left\| \hat{J}_\pm |\alpha, j, m\rangle \right\|^2 = \langle \alpha, j, m | \hat{J}_\mp \hat{J}_\pm | \alpha, j, m \rangle = \hbar^2 (j^2 + j - m^2 \mp m), \quad (195)$$

while their phases can be set to zero by adjusting the overall phases of the basis  $|\alpha, j, m\rangle$  states. This gives us

$$\hat{J}_\pm |\alpha, j, m\rangle = \hbar \sqrt{j^2 + j - m^2 \mp m} \times |\alpha, j, m \pm 1\rangle. \quad (196)$$

and hence matrix elements

$$\begin{aligned} \langle \alpha', j', m' | \hat{J}_z | \alpha, j, m \rangle &= \delta_{\alpha', \alpha} \delta_{j', j} \times \delta_{m', m} \times \hbar m, \\ \langle \alpha', j', m' | \hat{J}_+ | \alpha, j, m \rangle &= \delta_{\alpha', \alpha} \delta_{j', j} \times \delta_{m', m+1} \times \hbar \sqrt{j^2 + j - m^2 - m}, \\ \langle \alpha', j', m' | \hat{J}_- | \alpha, j, m \rangle &= \delta_{\alpha', \alpha} \delta_{j', j} \times \delta_{m', m-1} \times \hbar \sqrt{j^2 + j - m^2 + m}. \end{aligned} \quad (197)$$

Note that all the matrix elements here are block-diagonal: they are diagonal WRT  $\alpha$  and  $j$ , but not  $m$ . Thus, the diagonal blocks of states with the same  $\alpha$  and  $j$  but different  $m$  form *multiplet of the angular momentum algebra*, each multiplet comprising  $(2j+1)$  states for  $m = -j, \dots, +j$ . In other words, the quantum numbers  $\alpha$  and  $j$  label different multiplets of the angular momentum algebra, while  $m$  labels the states within the  $(\alpha, j)$  multiplet.

Furthermore, the matrix elements (197) do not depend on  $\alpha$ . Thus, all the multiplets  $(\alpha, j)$  with the same  $j$  but different  $\alpha$ 's are of the same *multiplet type*. In other words,  $j$  specifies the multiplet type while  $\alpha$  labels different multiplets of states of the same type  $j$ . From the Lie algebra point of view, this means that  $j$  — but not  $\alpha$  — labels different irreducible representations of the angular momentum algebra.

Specifically, for each integer or half integer  $j \geq 0$ , the representation  $(j)$  comprises three  $(2j + 1) \times (2j + 1)$  matrices whose elements follow from eqs. (197):

$$\begin{aligned} (J_z^{(j)})_{m',m} &= \delta_{m',m} \times \hbar m, \\ (J_+^{(j)})_{m',m} &= \delta_{m',m+1} \times \hbar \sqrt{j^2 + j - m^2 - m}, \\ (J_-^{(j)})_{m',m} &= \delta_{m',m-1} \times \hbar \sqrt{j^2 + j - m^2 + m}, \end{aligned} \quad (198)$$

and hence

$$\begin{aligned} (J_x^{(j)})_{m',m} &= \frac{1}{2}(J_+^{(j)})_{m',m} + \frac{1}{2}(J_-^{(j)})_{m',m}, \\ (J_y^{(j)})_{m',m} &= -\frac{i}{2}(J_+^{(j)})_{m',m} + \frac{i}{2}(J_-^{(j)})_{m',m}. \end{aligned} \quad (199)$$

In terms of these matrices, the matrix elements (197) of the angular momentum operators can be summarized as

$$\langle \alpha', j', m' | \hat{J}_i | \alpha, j, m \rangle = \delta_{\alpha', \alpha} \delta_{j', j} \times (J_i^{(j)})_{m',m} \quad \text{for } i = x, y, z. \quad (200)$$

Consequently, the finite  $(2j + 1) \times (2j + 1)$  matrices  $J_i^{(j)}$  are Hermitian and obey the same commutation relations as the angular momentum operators,

$$[J_i^{(j)}, J_k^{(j)}] = i\hbar \epsilon_{ij\ell} J_\ell^{(j)}, \quad (201)$$

which confirm that they indeed represent the angular momentum algebra.

Moreover, since we have obtained the spectrum of  $j$  and  $m$  and the matrix elements (197) for a completely general angular momentum generating rotations of a most general quantum system, it follows that *the representations  $(j)$  for  $j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$  comprise a complete list of all finite irreducible representations of the angular momenta algebra.*



But for any particular quantum system, its Hilbert space may contain multiplets in some representations ( $j$ ) but not in other representations. Likewise, the spectrum of multiplets ( $\alpha, j$ ) for each allowed representation ( $j$ ) depends on the specifics of the system in question. For example, for a spinless particle in a central potential the only allowed values of  $j = \ell$  are integers  $\ell = 0, 1, 2, 3, \dots$ , but for each  $\ell$  there can be infinitely many multiplets  $(n_r, \ell)$  distinguished by their radial quantum numbers  $n_r$ . On the other hand, the spin states of an elementary particle form a single irreducible multiplet ( $j = s$ ), but the spin value  $s$  can be integer or half-integer; for example, the electrons, the protons, and the neutrons all have  $s = \frac{1}{2}$ . The only hard rule which applies to all quantum systems with a rotational symmetry is that every existing  $(\alpha, j)$  multiplet must have all of the  $2j + 1$  states  $|\alpha, j, m\rangle$  for all  $m = -j, \dots, +j$ .

Now let's go back to the general quantum system and the abstract representations of the angular momentum. A few sections above, we have learned that a representation of the Lie algebra is a representation of the corresponding Lie group and vice versa. In particular, an irreducible representation of the angular momentum algebra is an irreducible representation of the rotation group  $SO(3)$  according to

$$\mathcal{D}_{m',m}^{(j)}(\mathbf{n}, \phi) = \left( \text{matrix } \exp\left(\frac{-i\phi}{\hbar} \mathbf{n} \cdot \mathbf{J}^{(j)}\right) \right)_{m',m}. \quad (202)$$

These  $\|\mathcal{D}^{(j)}(\mathbf{n}, \phi)\|$  are unitary  $(2j + 1) \times (2j + 1)$  matrices, and their matrix products follow the group product of the rotation symmetries: For any 2 rotations  $R_1$  and  $R_2$  and their product  $R_1 R_2 = R_3$ ,

$$\|\mathcal{D}^{(j)}(R_1)\| \times \|\mathcal{D}^{(j)}(R_2)\| = \|\mathcal{D}^{(j)}(R_3)\|, \quad (203)$$

or in terms of matrix elements

$$\sum_{m'} \mathcal{D}_{m'',m'}^{(j)}(R_1) \mathcal{D}_{m',m}^{(j)}(R_2) = \mathcal{D}_{m'',m}^{(j)}(R_3). \quad (204)$$

In the quantum mechanical context, the representations (202) are the diagonal blocks of the rotation operators  $\hat{\mathcal{R}}(\mathbf{n}, \alpha)$  in the  $|\alpha, j, m\rangle$  basis:

$$\hat{\mathcal{R}}(\mathbf{n}, \phi) |\alpha, j, m\rangle = \sum_{m'} |\alpha, j, m'\rangle \times \mathcal{D}_{m',m}^{(j)}(\mathbf{n}, \phi). \quad (205)$$

Let's take a closer look at the rotation matrices (202) for  $j = 0$ ,  $j = \frac{1}{2}$ , and  $j = 1$ . For  $j = 0$ , the generator matrices  $J_i^{(0)}$  are  $1 \times 1$ , so they are simply numbers; moreover, these numbers happen to be zero for all 3 generators, *cf.* eqs. (198). Consequently, the rotation matrices  $\mathcal{D}^{(0)}(R)$  are also  $1 \times 1$ , so they are simply numbers, and for all rotations  $R$  these numbers amount to  $\exp(0) = 1$ . Thus, the  $j = 0$  representation of the rotation group is *trivial*:

$$\|\mathcal{D}^{(0)}(R)\| \equiv 1 \quad \forall R, \quad (206)$$

and the rotations have no effect whatsoever. Consequently, quantum states  $|\alpha, j = 0, m = 0\rangle$  are invariant under all space rotations.

The simplest non-trivial representation of the rotation group obtains for  $j = \frac{1}{2}$ . In this case, the generator matrices (198), (199) and the rotation matrices (202) are  $2 \times 2$ . Specifically,

$$\|J_x^{(1/2)}\| = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \|J_y^{(1/2)}\| = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}, \quad \|J_z^{(1/2)}\| = \frac{\hbar}{2} \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (207)$$

or in terms of the Pauli matrices

$$\|J_i^{(1/2)}\| = \frac{\hbar}{2} \sigma_i, \quad (208)$$

hence

$$\|\mathcal{D}^{(1/2)}(\mathbf{n}, \phi)\| = \exp\left(-\frac{i}{2}\phi\mathbf{n} \cdot \vec{\sigma}\right) = \cos\frac{\phi}{2} \mathbf{1}_{2 \times 2} - i \sin\frac{\phi}{2} n_i \sigma_i. \quad (209)$$

As you should have seen in [homework set#9](#), problem 1(d-f), these matrices indeed form a representation of the rotation symmetry. Moreover, this representation gives rise to the Cayley–Klein formula for calculating a product of two rotations: it is easier to multiply the  $2 \times 2$  matrices (209) than the  $SO(3)$  matrices  $R_{ij}(\mathbf{n}, \phi)$  themselves.

Finally, in the  $j = 1$  representation, the  $3 \times 3$  rotation matrices  $\mathcal{D}_{m',m}^{(1)}(R)$  are equivalent

to the  $SO(3)$  rotations  $R$  themselves, but written in terms of the complex coordinates

$$\begin{aligned}\xi_{+1} &= \frac{-x - iy}{\sqrt{2}}, \\ \xi_0 &= z, \\ \xi_{-1} &= \frac{+x - iy}{\sqrt{2}},\end{aligned}\tag{210}$$

instead of the usual  $(x, y, z)$  coordinates. Thus, for any rotation  $R(\mathbf{n}, \phi)$

$$x'_i = \sum_j R_{ij}(\mathbf{n}, \phi) \times x_j \iff \xi'_{m'} = \sum_m \xi_m \times \mathcal{D}_{m,m'}^{(1)}(\mathbf{n}, \phi).\tag{211}$$

To how this works, note that the  $SO(3)$  matrices  $R_{ij}(\mathbf{n}, \phi)$  themselves are generated by the

$$(\tilde{J}_k)_{ij} = i\hbar\epsilon_{ikj},\tag{212}$$

or in explicit matrix form

$$\|\tilde{J}_x\| = \hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & +i & 0 \end{pmatrix}, \quad \|\tilde{J}_y\| = \hbar \begin{pmatrix} 0 & 0 & +i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad \|\tilde{J}_z\| = \hbar \begin{pmatrix} 0 & -i & 0 \\ +i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},\tag{213}$$

thus

$$R_{ij}(\mathbf{n}, \phi) = \left( \exp\left(\frac{-i\phi}{\hbar} \mathbf{n} \cdot \tilde{\mathbf{J}}\right) \right)_{ij}.\tag{214}$$

At the same time, eqs. (198) and (199) for the  $j = 1$  representation of the angular momenta give us

$$\|J_x^{(1)}\| = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \|J_y^{(1)}\| = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & +i & 0 \\ -i & 0 & +i \\ 0 & -i & 0 \end{pmatrix}, \quad \|J_z^{(1)}\| = \hbar \begin{pmatrix} +1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},\tag{215}$$

and with a bit of tedious algebra one can show that for each of these 3 matrices

$$\|J_k^{(1)}\| = \|W\| \times \|\tilde{J}_k\| \times \|W\|^{-1}\tag{216}$$

— or in index notations

$$(J_k^{(1)})_{m',m} = \sum_{i,j} W_{m',i} (\tilde{J}_k)_{ij} (W^{-1})_{j,m}\tag{217}$$

— where  $\|W\|$  is the matrix which translates from the real coordinates  $(x, y, z)$  to the complex

coordinates  $(\xi_{+1}, \xi_0, \xi_{-1})$ . Consequently,

$$\begin{aligned}
\|\mathcal{D}^{(1)}(\mathbf{n}, \phi)\| &= \exp\left(\frac{-i\phi}{\hbar}\mathbf{n} \cdot \left(\|\mathbf{J}^{(1)}\| = \|W\| \|\tilde{\mathbf{J}}\| \|W\|^{-1}\right)\right) \\
&= \|W\| \exp\left(\frac{-i\phi}{\hbar}\mathbf{n} \cdot \|\tilde{\mathbf{J}}\|\right) \|W\|^{-1} \\
&= \|W\| \|R(\mathbf{n}, \phi)\| \|W\|^{-1},
\end{aligned} \tag{218}$$

which means that the  $(j = 1)$  representation matrices  $\|\mathcal{D}^{(1)}(\mathbf{n}, \phi)\|$  are indeed equivalent to the  $SO(3)$  rotation matrices  $\|R(\mathbf{n}, \phi)\|$  translated to the complex coordinates  $\xi_m$ . Therefore, **the  $(j = 1)$  representation itself is said to be *equivalent* to the vector representation of the 3D rotation group.**

In a similar manner, for any integer  $j$  the  $(j)$  representation is equivalent to a tensor representation of the rotation group; specifically, to the representation by  $j$ -index tensors which are totally symmetric in all  $j$  indices and have zero ‘traces’,

$$\begin{aligned}
T_{i_1, i_2, \dots, i_j} &= +T_{\text{any permutation of } i_1, i_2, \dots, i_j}, \\
\sum_k T_{k, k, i_3, \dots, i_j} &= 0 \quad \forall i_3, \dots, i_j.
\end{aligned} \tag{219}$$

Indeed, such tensors have  $(2j + 1)$  independent components, so all the  $T_{i_1, \dots, i_j}$  can be written as linear combinations of the *spherical tensor components*  $T_m$  (for  $m = -j, \dots, +j$ ) which transform under the rotation symmetries as

$$T'_{m'} = \sum_m T_m \times \mathcal{D}_{m, m'}^{(j)}. \tag{220}$$

I shall return to such spherical tensor components later in class, as they play important role in the [Wigner–Echard theorem](#).

## ROTATION GROUPS $SO(3)$ AND $Spin(3)$

As far as the particle positions and other space degrees of freedom are concerned, a rotation through angle  $2\pi$  around any axis brings everything back to the initial configuration. And indeed, the  $SO(3)$  matrix for any  $2\pi$  rotation is a unit matrix:

$$R_{ij}(\mathbf{n}, \phi) = \cos \phi \delta_{ij} + \sin \phi n_k \epsilon_{ikj} + (1 - \cos \phi) n_i n_j \longrightarrow \delta_{ij} \text{ for } \phi = 2\pi. \quad (221)$$

However, when we look at various ( $j$ ) representations of the rotation group, we find that

$$\mathcal{D}_{m',m}^{(j)}(\mathbf{n}, 2\pi) = \delta_{m',m} \times (-1)^{2j}, \quad (222)$$

or in other words

$$\begin{aligned} \|\mathcal{D}^{(j)}(\mathbf{n}, 2\pi)\| &= +1_{(2j+1) \times (2j+1)} \quad \text{for integer } j, \\ \|\mathcal{D}^{(j)}(\mathbf{n}, 2\pi)\| &= -1_{(2j+1) \times (2j+1)} \quad \text{for half-integer } j. \end{aligned} \quad (223)$$

For example, for  $j = \frac{1}{2}$

$$\|\mathcal{D}^{(1/2)}(\mathbf{n}, 2\pi)\| = \exp\left(\frac{-2\pi i}{2} \mathbf{n} \cdot \vec{\sigma}\right) = -1_{2 \times 2} \quad (224)$$

because for any axis  $\mathbf{n}$ , the matrix  $\mathbf{n} \cdot \vec{\sigma}$  has eigenvalues  $\pm 1$  and  $\exp(\mp \pi i) = -1$ .

To verify eqs. (222) and (223), let's start with a  $2\pi$  rotation around the  $z$  axis:

$$\begin{aligned} \mathcal{D}_{m',m}^{(j)}(z \text{ axis}, 2\pi) &= \left( \exp\left(\frac{-2\pi i}{\hbar} J_z^{(j)}\right) \right)_{m',m} \\ &\quad \langle\langle \text{since the } J_z^{(j)} \text{ matrix is diagonal in the } |j, m\rangle \text{ basis} \rangle\rangle \\ &= \delta_{m',m} \times \exp\left(\frac{-2\pi i}{\hbar} \times \hbar m\right) \\ &= \delta_{m',m} \times \exp(-2\pi i m), \end{aligned} \quad (225)$$

where for integer or half-integer  $m$

$$\exp(2\pi i m) = (-1)^{2m} = (-1)^{2j}, \quad (226)$$

hence

$$\|\mathcal{D}^{(j)}(z \text{ axis}, 2\pi)\| = (-1)^{2j} \times \text{unit matrix.} \quad (227)$$

For rotations around other axes  $\mathbf{n}$ , we use

$$R(\mathbf{n}, \phi) = \tilde{R}^{-1} \times R(z \text{ axis}, \phi) \times \tilde{R} \quad (228)$$

where  $\tilde{R}$  is the rotation which turns  $\mathbf{n}$  into  $(0, 0, 1)$ .

Consequently,

$$\begin{aligned} \|\mathcal{D}^{(j)}(\mathbf{n}, 2\pi)\| &= \|\mathcal{D}^{(j)}(\tilde{R})\|^{-1} \times \|\mathcal{D}^{(j)}(z \text{ axis}, 2\pi)\| \times \|\mathcal{D}^{(j)}(\tilde{R})\| \\ &= \|\mathcal{D}^{(j)}(\tilde{R})\|^{-1} \times (-1)^{2j} \times 1 \times \|\mathcal{D}^{(j)}(\tilde{R})\| \\ &= (-1)^{2j} \times 1, \end{aligned} \quad (229)$$

just like for the  $2\pi$  rotation around the  $z$  axis. The bottom line is: **For integer  $j$ , the rotation by  $2\pi$  act trivially, but for half-integer  $j$  they are represented by the non-trivial  $-1$  matrices.**

However, the rotations through  $4\pi$  around any axis act trivially for all  $j$  because

$$\|\mathcal{D}^{(j)}(\mathbf{n}, 4\pi)\| = \|\mathcal{D}^{(j)}(\mathbf{n}, 2\pi)\|^2 = (-1)^{4j} \times 1, \quad (230)$$

and  $(-1)^{4j} = +1$  for any integer or half-integer  $j$ .

From the  $SO(3)$  group's point of view, this means that for the half-integer  $j$  representations, the same  $SO(3)$  matrix  $R_{ij}(\mathbf{n}, \phi) = R_{ij}(\mathbf{n}, \phi + 2\pi)$  is represented by two distinct  $(2j + 1) \times (2j + 1)$  matrices which differ in the overall sign

$$\|\mathcal{D}^{(j)}(\mathbf{n}, \phi)\| \quad \text{and} \quad \|\mathcal{D}^{(j)}(\mathbf{n}, \phi + 2\pi)\| = -\|\mathcal{D}^{(j)}(\mathbf{n}, \phi)\| \quad (231)$$

because

$$\|\mathcal{D}^{(j)}(\mathbf{n}, \phi + 2\pi)\| = \|\mathcal{D}^{(j)}(\mathbf{n}, 2\pi)\| \times \|\mathcal{D}^{(j)}(\mathbf{n}, \phi)\| = (-1)^{2j} \|\mathcal{D}^{(j)}(\mathbf{n}, \phi)\| \quad (232)$$

where  $(-1)^{2j} = -1$ . In other words, the representations with half-integer  $j$  are *double-valued representations* of the  $SO(3)$  rotation group. On the other hand, in representations with integer  $j$  and hence  $(-1)^{2j} = +1$ , we have

$$\|\mathcal{D}^{(j)}(\mathbf{n}, \phi + 2\pi)\| = +\|\mathcal{D}^{(j)}(\mathbf{n}, \phi)\| \quad (233)$$

so these are single-valued representations of the  $SO(3)$ .

This is an example of a general problem for many Lie groups: A representation of the Lie Algebra always generates a representation of the corresponding Lie group, but some of these representations may be multi-valued rather than single-valued. And the general solution to this problem is to replace the original Lie group  $G$  with its *universal covering group*  $G'$  such that the map between  $G$  and  $G'$  preserves the group product but several elements of  $G'$  corresponds to the same element of  $G$ , and all the multi-valued representations of  $G$  become single-valued in terms of the  $G'$ .

In particular, for the rotations in 3D we need to replace the  $SO(3)$  group with its double covering group called  $Spin(3)$ . Thus, every  $SO(3)$  matrix  $R_{ij}$  corresponds to two distinct elements  $\pm M(R)$  of the  $Spin(3)$  group, but the map in the other direction is single valued

$$\pm M(R) \rightarrow \text{same } R_{ij}. \quad (234)$$

In rotation terms,  $\pm M(\mathbf{n}, \phi)$  distinguish between rotations through angles  $\phi$  and  $\phi + 2\pi$ :

$$M(\mathbf{n}, \phi + 2\pi) = -M(\mathbf{n}, \phi). \quad (235)$$

In particular, a rotation by  $2\pi$  around any axis corresponds to  $M = -1$  rather than  $M = +1$ , but a rotation by  $4\pi$  is trivial and corresponds to  $M = +1$ .

As a group,  $Spin(3)$  is isomorphic to the  $SU(2)$  — the group of  $2 \times 2$  unitary matrices of unit determinant. Indeed, any  $SU(2)$  matrix can be written in the form

$$M = \begin{pmatrix} a - ib_z & -ib_x - b_y \\ -ib_x + b_y & a + ib_z \end{pmatrix} \quad \text{for real } a, b_x, b_y, b_z, \quad a^2 + b_x^2 + b_y^2 + b_z^2 = 1. \quad (236)$$

Equivalently, we may identify

$$a = \cos \frac{\phi}{2}, \quad \mathbf{b} = \sin \frac{\phi}{2} \mathbf{n} \quad (237)$$

for a real phase  $\phi$  defined modulo  $4\pi$  (but not modulo  $2\pi$ ) and a real unit vector  $\mathbf{n}$ . In terms of these parameters,

$$M(\mathbf{n}, \phi) = \cos \frac{\phi}{2} - i \sin \frac{\phi}{2} \mathbf{n} \cdot \vec{\sigma} = \exp(-i \frac{\phi}{2} \mathbf{n} \cdot \vec{\sigma}). \quad (238)$$

Conversely, for any unit vector  $\mathbf{n}$  and any phase  $\phi$  eq. (238) defines an  $SU(2)$  matrix. As you should have seen in [homework set#9](#), every such  $SU(2)$  matrix  $M$  maps to an  $SO(3)$

rotation matrix  $R_{ij}(M)$  according to

$$M^\dagger \sigma_i M = R_{ij}(M) \sigma_j, \quad (239)$$

and this map is  $2 \rightarrow 1$ : both  $+M$  and  $-M$  map to the same  $R_{ij}(M)$ . Moreover, for  $M(\mathbf{n}, \phi)$  as in eq. (238),

$$R_{ij}(M(\mathbf{n}, \phi)) = \text{rotation matrix } R_{ij}(\mathbf{n}, \phi). \quad (240)$$

so the  $SU(2)$  matrices indeed provide the double cover of the  $SO(3)$  rotation group, thus  $\text{Spin}(3) \cong SU(2)$ .

In the opposite direction  $R_{ij} \rightarrow M(R)$ , the  $2 \times 2$  matrix  $M$  can be identified with the  $j = \frac{1}{2}$  representation  $\|\mathcal{D}^{(1/2)}(R)\|$ . As we have seen a few pages above, the  $j = \frac{1}{2}$  representation is double valued in terms of  $R$  but becomes single-valued in terms of  $M$ :

$$\|\mathcal{D}^{(1/2)}(\mathbf{n}, \phi + 2\pi)\| = -\|\mathcal{D}^{(1/2)}(\mathbf{n}, \phi)\| \quad \text{because} \quad M(\mathbf{n}, \phi + 2\pi) = -M(\mathbf{n}, \phi). \quad (241)$$

Likewise, all other representations of with half-integer  $j$  are double-valued representations of the  $SO(3)$  group but become single-valued representations of its double cover  $SU(2)$ ,

$$\forall M \in SU(2) \quad \exists \text{ unique } \|\mathcal{D}^{(j)}(M)\|. \quad (242)$$

And of course, all integer- $j$  representations of the  $SO(3)$  group are also single-valued in terms of the  $SU(2)$ . Indeed, in the [homework set#10](#) you shall see that all the matrix elements of any representation  $j$  of the  $\text{Spin}(3)$  symmetry are polynomials of degree  $2j$  of the  $SU(2)$  matrix elements,

$$\mathcal{D}_{m',m}^{(j)}(M) = \text{polynomial}[\text{degree} = 2j](M_{11}, M_{12}, M_{21}, M_{22}). \quad (243)$$

Let me conclude this section with the geometries of the  $SO(2)$ ,  $SO(3)$ , and  $\text{Spin}(3)$  group manifolds. The manifold of the 2D rotation group  $SO(2)$  is a unit circle  $S^1$ . To see that, let's identify the 2D plane  $(x, y)$  with the complex plane of  $z = x + iy$ . In terms of  $z$ , a rotation through angle  $\alpha$  acts by multiplication as

$$R(\alpha) z = e^{i\alpha} z, \quad (244)$$

where the unimodular complex numbers  $e^{i\alpha}$  span a unit circle.



The manifold of the  $\text{Spin}(3) \cong \text{SU}(2)$  rotation group is  $S^3$ , a unit 3D sphere spanned by unit vectors in a 4D space. To see that, note that

$$\forall \text{ unit 4-vector } (a, b_x, b_y, b_z), \quad a^2 + b_x^2 + b_y^2 + b_z^2 = 1,$$

$$M = \begin{pmatrix} a - ib_z & -ib_x - b_y \\ -ib_x + b_y & a + ib_z \end{pmatrix} \text{ is an } \text{SU}(2) \text{ matrix,} \quad (245)$$

and conversely, any  $\text{SU}(2)$  matrix can be written in this form for a unique unit 4-vector  $(a, b_x, b_y, b_z)$ . Treating these 4-vectors as radius vectors in some 4D space, we see that they span a unit sphere  $S^3$ , thus the group manifold of  $\text{Spin}(3) \cong \text{SU}(2)$  is indeed  $S^3$ .

The manifold of the  $\text{SO}(3)$  rotation group is more complicated. Every  $\text{SO}(3)$  matrix  $R_{ij}$  corresponds to a pair of  $\text{SU}(2)$  matrices  $\pm M(R)$  which differ in overall sign. In terms of the  $\text{SU}(2)$  group manifold, this means that every  $\text{SO}(3)$  matrix corresponds to a pair of diametrically opposed points on the 3-sphere  $S^3$ . However, both of these points — but no other point on the  $S^3$  — lie on the same straight line through the center of the sphere. Thus, the space of the  $\text{SO}(3)$  matrices is isomorphic to the space of straight lines in 4D going through the center.

In [projective geometry](#), straight lines through a fixed center are used to project a 3D object onto a 2D plane. And in order to accommodate the lines that are parallel to the projection plane, the 2D plane is augmented with an extra semi-circle of points at infinity. Such augmented plane is called the *projective plane*  $\mathbf{RP}^2$ .

This construction can be generalized to higher dimensions. In particular, in 4D the straight lines through the center project a 4D object onto a 3D hyperplane. Again, to accommodate the lines parallel to that hyperplane, we augment it with a 2D hemisphere of extra points at infinite distance, and such augmented 3D hyperplane becomes the *3D projective space*  $\mathbf{RP}^3$ . And this 3D projective space  $\mathbf{RP}^3$  is our best description of the  $\text{SO}(3)$  group manifold.

Geometries of the rotations groups  $\text{Spin}(d)$  and  $\text{SO}(d)$  in higher space dimensions  $d > 3$  are much more complicated; in particular, they are not higher-dimensional spheres or projective spaces. But fortunately, we do not need their geometries for this class.

## Orbital Angular Momentum and Spin

A few pages above I stated that for any rotationally symmetric quantum system, any  $(\alpha, j)$  multiplet of the symmetry must have all of the  $(2j + 1)$  states for all  $m = -j, \dots, +j$ ; but the spectrum of the multiplets  $(\alpha, j)$  depends on a particular quantum system. Most generally,  $j$  must be a non-negative integer or a positive half-integer, but it does not have to take all of these values; instead, a particular system may have a much more restricted spectrum of  $j$ . In this section we shall see two examples of such restricted spectrum of  $j$ : the orbital angular momentum, and the spin.

### ORBITAL ANGULAR MOMENTUM

For simplicity, consider a single spinless particle in a central potential,

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2M} + V(\hat{r}). \quad (246)$$

This system has a rotational symmetry generated by the orbital angular momentum  $\hat{\mathbf{J}} = \hat{\mathbf{L}} = \hat{\mathbf{x}} \times \hat{\mathbf{p}}$ . For this orbital angular momentum, the only allowed values of  $j = \ell$  are integers; the half-integral  $\ell$  are forbidden. On the other hand, all integral values of  $\ell = 0, 1, 2, 3, \dots$  are allowed, and for each such  $\ell$  there are infinitely many distinct multiplets of states  $|n_r, \ell, m\rangle$  distinguished by their radial quantum numbers  $n_r$ .

To see how this works, note that the wave-function  $\Psi(x, y, z)$  of the particle in question depends only on its space coordinates, and it must be a single-valued function of these coordinates. Consequently, a rotation by  $2\pi$  — which leaves the coordinates unchanged — must act trivially on this wave-function, thus

$$\hat{\mathcal{R}}(\mathbf{n}, 2\pi) |\Psi\rangle = + |\Psi\rangle, \quad (247)$$

which immediately restricts the rotation multiplets  $(\alpha, m)$  to the representations  $(j)$  where  $R(2\pi) = +1$  rather than  $-1$ . And that's why  $\ell$  should be integer rather than half-integer.

Next, let's rewrite the Hamiltonian (246) as

$$\hat{H} = \frac{\hat{p}_r^2}{2M} + \frac{\hat{\mathbf{L}}^2}{2M\hat{r}^2} + V(\hat{r}) \quad (248)$$

(*cf.* [homework set#4](#), problem 2(f)) and seek its eigenstates using the separation of variables

method in spherical coordinates. Thus, we look for eigenfunctions of the form

$$\Psi(r, \theta, \phi) = \psi(r) \times Y(\theta, \phi) \quad (249)$$

where

$$\hat{\mathbf{L}}^2 Y(\theta, \phi) = \ell(\ell + 1)\hbar^2 Y(\theta, \phi) \quad (250)$$

and

$$\left( -\frac{\hbar^2}{2M} \frac{d^2}{dr^2} + \frac{\ell(\ell + 1)\hbar^2}{2Mr^2} + V(r) \right) (r\psi(r)) = E \times r\psi(r). \quad (251)$$

As everybody learns in the undergraduate school, eq. (250) has  $2\ell + 1$  independent solutions for each integer  $\ell = 0, 1, 2, 3, \dots$ , and we may label these solutions by  $m = -\ell, \dots, +\ell$  according to the eigenstates  $\hbar m$  of the  $\hat{L}_z$  operator. At the same time, for any given  $\ell$ , the radial equation (251) has infinitely many eigenstates labeled by the radial quantum number  $n_r$ . Depending on the potential's behavior for  $r \rightarrow 0$  and for  $r \rightarrow \infty$ , the energy spectrum of radial Hamiltonian can be discrete, continuous, or mixed, but in light of the boundary condition  $r\psi(r) = 0$  for  $r = 0$ , this spectrum (for a given  $\ell$ ) should be non-degenerate WRT  $n_r$ .

Going back to the full 3D Hamiltonian, we find it has a basis of eigenstates  $|n_r, \ell, m\rangle$  with wave-functions

$$\Psi_{n_r, \ell, m}(r, \theta, \phi) = \psi_{n_r, \ell}(r) \times Y_{\ell, m}(\theta, \phi) \quad (252)$$

and energies  $E(n_r, \ell)$  which do not depend on  $m$ ,

$$\hat{H} |n_r, \ell, m\rangle = E(n_r, \ell) |n_r, \ell, m\rangle \quad (253)$$

because  $m$  — unlike  $\ell$  — does not enter the radial equation (251). Thus, each energy level  $E(n_r, \ell)$  has  $(2\ell + 1)$ -fold degeneracy.

For most potentials  $V(r)$ , the discrete part of the energy spectrum has no further degeneracy — there are no coincidences between  $E(n_r, \ell)$  for different  $(n_r, \ell)$ , except by accident. But for the Coulomb potential  $V(r) = -Ze^2/r$  and for the harmonic potential  $V(r) = (m\omega^2/2)r^2$  the energies have much larger degeneracies:

- For the Coulomb potential, the bound state energies depend only on the principle quantum number  $N = n_r + 1 + \ell = 1, 2, 3, \dots$ , regardless how it's apportioned between  $n_r$  and  $\ell$ ,

$$E(n_r, \ell) = E(N \text{ only}) = -\frac{Me^4 Z^2}{2\hbar^2} \times \frac{1}{N^2}. \quad (254)$$

- For the harmonic potential, all states are bound, and their energies also depends on a single combination of  $n_r$  and  $\ell$ , this time on  $N = 2n_r + \ell = 0, 1, 2, 3, \dots$ ,

$$E(n_r, \ell) = E(N \text{ only}) = \hbar\omega\left(\frac{3}{2} + N\right). \quad (255)$$

In both cases, the extra degeneracy is not an accident but a consequence of a larger symmetry group  $G$  which contains the rotational symmetry as a subgroup: For the Coulomb potential  $G = SU(2) \times SU(2) \cong \text{Spin}(4)$ , while for the harmonic potential  $G = SU(3)$ . I am going to defer the analysis of the Coulomb case to the [next homework set#11](#), while in these notes I focus on the harmonic case.

A simple way to analyze the 3D harmonic oscillator is to realize that it's equivalent to a system of 3 independent 1D harmonic oscillators of the same frequency  $\omega$ :

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2M} + \frac{M\omega^2}{2}\hat{r}^2 = \sum_{i=x,y,z} \left( \frac{\hat{p}_i^2}{2M} + \frac{M\omega^2}{2}\hat{x}_i^2 \right), \quad (256)$$

and hence

$$\hat{H} = \sum_{i=x,y,z} \hbar\omega\left(\frac{1}{2} + \hat{a}_i^\dagger \hat{a}_i\right) \quad (257)$$

where

$$\hat{a}_i = \frac{M\omega\hat{x}_i + i\hat{p}_i}{\sqrt{2\hbar\omega M}} \quad \text{and} \quad \hat{a}_i^\dagger = \frac{M\omega\hat{x}_i - i\hat{p}_i}{\sqrt{2\hbar\omega M}} \quad (258)$$

obey the commutation relations

$$[\hat{a}_i, \hat{a}_j] = 0, \quad [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0, \quad [\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}. \quad (259)$$

We have dealt with the multi-oscillator systems earlier in class, so let me simply summarize the spectrum of the Hamiltonian (257): The eigenstates have form  $|n_x, n_y, n_z\rangle$  where each

$n_i$  takes non-negative integer values regardless of the other  $n_j$ ,

$$n_x, n_y, n_z = 0, 1, 2, \dots, \quad (260)$$

and the energies are given by a simple formula

$$E(n_x, n_y, n_z) = \sum_{i=x,y,z} \hbar\omega\left(\frac{1}{2} + n_i\right). \quad (261)$$

And since all 3 oscillators have the same frequency  $\omega$ , the energy depends only on the net number of quanta in all 3 oscillators,

$$N = n_x + n_y + n_z, \quad (262)$$

$$E(N) = \hbar\omega\left(\frac{3}{2} + N\right). \quad (263)$$

Moreover, due to equal frequencies of all 3 oscillators, the 9 operators

$$\hat{T}_{ij} = \hat{a}_i^\dagger \hat{a}_j, \quad i, j = x, y, z \quad (264)$$

commute with the Hamiltonian and hence generate a rather large symmetry group. Actually, one combination of the 9 operators (264) — the trace

$$\text{tr}(\hat{T}) = \hat{T}_{xx} + \hat{T}_{yy} + \hat{T}_{zz} = \hat{N} \quad (265)$$

— commutes with all the other operators (264), so it generates a separate abelian phase symmetry. But the remaining 8 operators (or rather 8 independent combinations of the operators (264)) generate a symmetry group isomorphic to  $SU(3)$  — the group of complex  $3 \times 3$  matrices which are unitary and have a unit determinant.

The representation theory of the  $SU(3)$  group is beyond the scope of this class, so let me simply state how the  $SU(3)$  symmetry acts on the creation operators and the  $N$ -quanta

states

$$|N : i_1, \dots, i_N\rangle \propto \hat{a}_{i_1}^\dagger \cdots \hat{a}_{i_N}^\dagger |\text{ground}\rangle : \quad (266)$$

An  $SU(3)$  matrix  $W_{ij}$  is represented by the unitary operator  $\hat{U}(W)$  such that

$$\hat{U}(W)\hat{a}_i^\dagger\hat{U}^\dagger(W) = \sum_j W_{ij}\hat{a}_j^\dagger \quad \text{while} \quad \hat{U}(W)|\text{ground}\rangle = |\text{ground}\rangle. \quad (267)$$

Consequently,

$$\begin{aligned} \hat{U}(W)\hat{a}_{i_1}^\dagger\hat{a}_{i_2}^\dagger\cdots\hat{a}_{i_N}^\dagger|\text{ground}\rangle &= \\ &= \hat{U}\hat{a}_{i_1}^\dagger\hat{U}^\dagger \times \hat{U}\hat{a}_{i_2}^\dagger\hat{U}^\dagger \times \cdots \times \hat{U}\hat{a}_{i_N}^\dagger\hat{U}^\dagger \times \hat{U}|\text{ground}\rangle \\ &= \left(\sum_{j_1} W_{i_1,j_1}\hat{a}_{j_1}^\dagger\right) \times \left(\sum_{j_2} W_{i_2,j_2}\hat{a}_{j_2}^\dagger\right) \times \cdots \times \left(\sum_{j_N} W_{i_N,j_N}\hat{a}_{j_N}^\dagger\right) \times |\text{ground}\rangle \\ &= \sum_{j_1,j_2,\dots,j_N} W_{i_1,j_1}W_{i_2,j_2}\cdots W_{i_N,j_N} \times \hat{a}_{j_1}^\dagger\hat{a}_{j_2}^\dagger\cdots\hat{a}_{j_N}^\dagger|\text{ground}\rangle, \end{aligned} \quad (268)$$

and hence the  $N$ -quanta states transform as  $N$ -index symmetric tensors,

$$\hat{U}(W)|N : i_1, \dots, i_N\rangle = \sum_{j_1,\dots,j_N} W_{i_1,j_1}\cdots W_{i_N,j_N}|N : j_1, \dots, j_N\rangle \quad (269)$$

From the  $SU(3)$  point of view, the rotation symmetry is the  $SO(3)$  subgroup of the  $SU(3)$  comprising the  $3 \times 3$  matrices which happen to be real (and hence orthogonal); this subgroup is generated by the

$$\hat{J}_i = i\hbar\epsilon_{ijk}\hat{T}_{jk} = i\hbar\epsilon_{ijk}\hat{a}_j^\dagger\hat{a}_k. \quad (270)$$

At each energy level  $E(N)$  of the 3D oscillator, there are  $\frac{1}{2}(N+1)(N+2)$  ways to apportion  $N$  between 3 non-negative integers  $n_x$ ,  $n_y$ , and  $n_z$ , hence  $\frac{1}{2}(N+1)(N+2)$  degenerate states. All these states form an irreducible multiplet of the  $SU(3)$  group, but it becomes reducible

from the  $SO(3)$  subgroup point of view. For example:

For $N = 0$ there is 1 state in	$(\ell = 0)$	multiplet of $SO(3)$ .
For $N = 1$ there are 3 states in	$(\ell = 1)$	multiplet of $SO(3)$ .
For $N = 2$ there are 6 states in	$(\ell = 2)$ and $(\ell = 0)$	multiplets of $SO(3)$ .
For $N = 3$ there are 10 states in	$(\ell = 3)$ and $(\ell = 1)$	multiplets of $SO(3)$ .
For $N = 4$ there are 15 states in	$(\ell = 4)$ , $(\ell = 2)$ , and $(\ell = 0)$	multiplets of $SO(3)$ .
For $N = 5$ there are 21 states in	$(\ell = 5)$ , $(\ell = 3)$ , and $(\ell = 1)$	multiplets of $SO(3)$ .
<i>etc., etc.</i>		

(271)

In general, for each  $N$  the values of  $\ell$  run down by 2 from  $N$  to 0 or 1,

$$\ell = N - 2k \quad \text{for integer } k = 0, 1, 2, \dots \text{ up to the integer part of } \frac{N}{2}. \quad (272)$$

Equivalently,

$$N = \ell + 2k \quad \text{where } k = 0, 1, 2, 3, \dots \quad \text{for each } \ell = 0, 1, 2, 3, \dots, \quad (273)$$

and we may reorganize the basis of states of definite energies from  $|n_x, n_y, n_z\rangle$  to  $|k, \ell, m\rangle$  where

$$N = n_x + n_y + n_z = \ell + 2k \quad \text{and} \quad E = \hbar\omega(N + \frac{3}{2}). \quad (274)$$

Physically, this  $k$  is the radial quantum number  $n_r$ , thus wavefunctions

$$\Psi_{k,\ell,m}(r, \theta, \phi) = \psi_{k,\ell}(r) \times Y_{\ell,m}(\theta, \phi). \quad (275)$$

From the purely radial point of view, the the states with different  $k$  and  $\ell$  but the same  $N = \ell + 2k$  have the same energies ‘by accident’. But from the 3-oscillator point of view, this degeneracy is no accident by the consequence of an enhanced symmetry group,  $SU(3)$  instead of  $SO(3)$ .

## SPIN

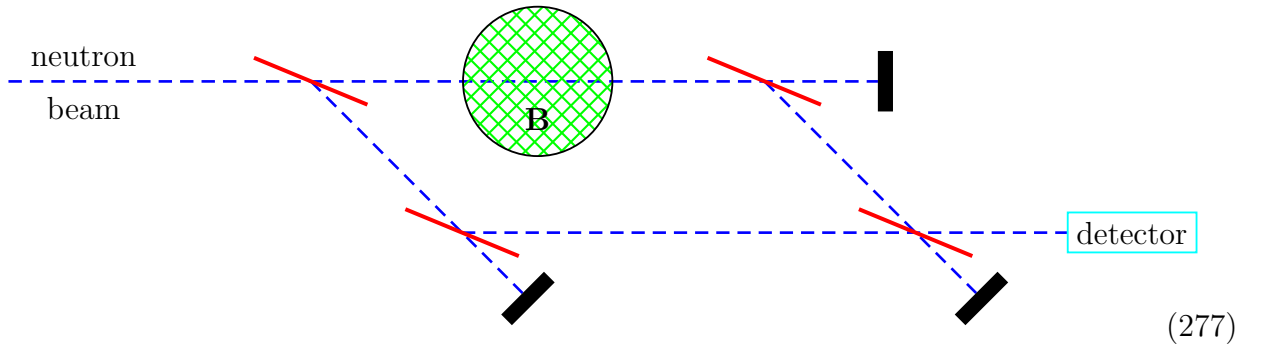
The spin degrees of freedom of an elementary particle usually comprise a single irreducible multiplet of spin states  $|s, m_s\rangle$  for a fixed  $s = j_{\text{spin}}$  while  $m_s = -s, \dots, +s$ . The value of  $s$  — called *the particle's spin* — depends on the particle species; for example, electrons, protons, and neutrons all have  $s = \frac{1}{2}$ . Consequently, each of these particles have 2 spin states with  $m_s = \pm\frac{1}{2}$ , and the spinor angular momentum acts in this 2-state Hilbert space as  $\hat{\mathbf{J}} = \frac{\hbar}{2}\vec{\sigma}$  (where  $\sigma_x, \sigma_y, \sigma_z$  are the Pauli matrices).

By the spin-statistics theorem, all integral spin particles are bosons while all half-integral spin particles are fermion. Thus, electrons, protons, and neutrons are fermions. Also, we have seen a rotation by  $2\pi$  acts differently in representations of integer and half-integer  $j$ ,

$$\hat{\mathcal{R}}(2\pi) = (-1)^{2j}. \quad (276)$$

Thus, for any boson, a rotation by  $2\pi$  acts trivially,  $\hat{\mathcal{R}}(2\pi) = 1$ . **But for a fermion  $\hat{\mathcal{R}}(2\pi) = -1$ , so a rotation by  $2\pi$  flips the overall phase of the particle's wave-function.**

By itself, the overall sign of the wave-function is not important. But it becomes important in the interference experiments where a particle may reach the same point via two different routes: In such a setup, flipping the wave-function sign for 1 of the routes changes a constructive interference into destructive and vice versa. For example, consider the neutron interference experiment like this:



where the red lines denote semi-transparent neutron mirrors and the green cross-hatched circle indicates the region between the poles of a magnet. The neutrons initially come from a nuclear reactor, but the Bragg diffraction off a crystal produces a secondary beam where all neutrons have the same speed. Consequently, all the neutrons take the same times  $t$  to traverse the magnet.



As a neutron flies by the magnet, the  $B$  field rotates its magnetic moment  $\vec{\mu}_N$  and hence its spin state with frequency  $\Omega \propto B$ . Altogether, the neutron's spin state is rotated through the angle  $\phi = \Omega t$ , which is proportional to the magnetic field with a known coefficient. Consequently, the experimentalists can directly control the value of the angle  $\phi$  and measure how the net flux at the detector as a function of  $\phi$ . And what they observe is:

- constructive interference for  $\phi = 0, 4\pi, 8\pi, \dots$ ,
- but destructive interference for  $\phi = 2\pi, 6\pi, 10\pi, \dots$

In particular, a rotation by  $\phi = 2\pi$  — which classically should have no effect — actually changes the interference from constructive to destructive and vice versa!

To conclude this section, let me say a few words about the net spin  $S$  of a composite body such as a nucleus or an atom. In general, this net spin depends on a particular state of the composite body. For example, the net spin of the three electrons in a lithium atom is  $S = \frac{1}{2}$  in the ground state, but some excited states have  $S = \frac{3}{2}$ . However, there is one general rule which applies to all states of any composite body: **if the net number of fermionic constituents of a body is even, then its net spin is always integer, and if the net number of fermionic constituents is odd then the net spin is half-integer**, thus

$$\hat{\mathcal{R}}(2\pi) = (-1)^{2S} = (-1)_{\text{fermion number}}. \quad (278)$$

For example, the net spin of all 8 electrons in an oxygen atom is always integer, while the net spin of all 7 electrons in a nitrogen atom is always half-integer. And if you include the nuclear spin, then the integrality of the net spin depends on a particular isotope. Thus, a helium-4 atom has integer net spin ( $S = 0$  in the ground state) while a helium-3 atom has a half-integer net spin ( $S = \frac{1}{2}$  in the ground state). Consequently, helium-4 atoms are bosons while helium-3 atoms are fermions, and the low-temperature quantum effects in the two isotopes of helium are very different!