

Supplement #1 to Lecture #27

Angular Momentum Eigenvalues (from lecture notes by Professor Dudley Herschbach)

Consider any Hermitian operator \underline{J} whose components satisfy the following commutation rules

$$[J_x, J_y] = i\hbar J_z$$

and the cyclic permutations thereof. Equivalently, the rules may be written as

$$\underline{J} \times \underline{J} = i\hbar \underline{J}$$

or as

$$[J_\ell, J_m] = i\hbar \sum_n \varepsilon_{\ell mn} J_n$$

where

$$\begin{aligned} \varepsilon_{\ell mn} &= +1 \text{ if } \ell, m, n \text{ are in cyclic order} \\ &= -1 \text{ if } \ell, m, n \text{ are in anti-cyclic order} \\ &= 0 \text{ if any two of } \ell, m, n \text{ are the same.} \end{aligned}$$

Seek to find eigenvalues λ for J^2 and μ for J_z such that

$$\begin{aligned} J^2 |\lambda\mu\rangle &= \lambda |\lambda\mu\rangle \\ J_z |\lambda\mu\rangle &= \mu |\lambda\mu\rangle. \end{aligned}$$

Since J^2 and J_z are Hermitian, λ and μ are real, and $|\lambda\mu\rangle$ are the simultaneous eigenvectors which render J^2 and J_z simultaneously diagonal.

First show $\lambda \geq \mu^2$

Proof: $\langle \lambda\mu | J^2 - J_z^2 | \lambda\mu \rangle = \lambda - \mu^2$

But

$$J^2 - J_z^2 = J_x^2 + J_y^2 + \cancel{J_z^2} - \cancel{J_z^2}$$

$$\begin{aligned} \lambda \mu J_x^2 |\lambda \mu\rangle &= \sum_{\lambda' \mu'} \langle \lambda \mu | J_x | \lambda' \mu' \rangle \underbrace{\langle \lambda' \mu' | J_x | \lambda \mu \rangle}_{\lambda \mu J_x^\dagger |\lambda' \mu'\rangle \text{ and } J_x^\dagger = J_x} \\ &= \sum_{\lambda' \mu'} |\langle \lambda \mu | J_x | \lambda' \mu' \rangle|^2 \rightarrow 0 \text{ and similarly for } J_y^2 \text{ term.} \end{aligned}$$

So

$$\lambda \mu J_x^2 + J_y^2 |\lambda \mu\rangle = \lambda - \mu^2 \geq 0 \quad \text{Q. E. D.}$$

Since $\mu^2 \geq 0$ this also implies $\lambda \geq 0$.

It is convenient to use the non-Hermitian operators

$$J_\pm = J_x \pm iJ_y \quad \text{Note } J_+^\dagger = J_-, J_-^\dagger = J_+.$$

These satisfy

$$\begin{aligned} [J_z, J_\pm] &= \pm \hbar J_\pm \quad \text{since } [J_z, J_x \pm iJ_y] = i\hbar J_y \pm i(-i\hbar J_x) \\ &= \hbar(J_x \pm iJ_y) = \hbar J_\pm. \end{aligned}$$

Apply this to $|\lambda \mu\rangle$ and find

$$(J_z J_\pm - J_\pm J_z) |\lambda \mu\rangle = \pm \hbar J_\pm |\lambda \mu\rangle$$

or

$$\begin{aligned} J_z(J_\pm |\lambda \mu\rangle) &= (J_\pm J_z \pm \hbar J_\pm) |\lambda \mu\rangle \\ &= (\mu \pm \hbar)(J_\pm |\lambda \mu\rangle) \quad \text{since } J_z |\lambda \mu\rangle = \mu |\lambda \mu\rangle. \end{aligned}$$

Thus $J_\pm |\lambda \mu\rangle$ is an eigenvector of J_z with eigenvalue $\mu \pm \hbar$. Hence J_+ “raises” the eigenvalue of μ to $\mu + \hbar$ and J_- “lowers” the eigenvalue of μ to $\mu - \hbar$.

Now note

$$[J^2, J_\pm] = 0$$

since J^2 commutes with its components J_x and J_y . Thus

$$J^2(J_\pm |\lambda \mu\rangle) = J_\pm \underbrace{J^2 |\lambda \mu\rangle}_{\lambda |\lambda \mu\rangle} = \lambda(J_\pm |\lambda \mu\rangle).$$

Thus $J_{\pm} |\lambda\mu\rangle$ remains an eigenvector of J^2 with the same eigenvalue λ as $|\lambda\mu\rangle$.

By repeated application of J_+ we can get eigenvectors with J_z eigenvalues of $\mu + \hbar, \mu + 2\hbar, \dots$ but the same eigenvalue λ of J^2 . Since $\mu^2 \geq \lambda$, for a given λ there must be some highest value of μ , call it μ_h , such that $J_+ |\lambda\mu_h\rangle = 0$ rather than generating a new eigenvector of still higher J_z -eigenvalue. Similarly, repeated application of J_- gives $\mu - \hbar, \mu - 2\hbar, \dots$ but would eventually violate $\mu^2 \leq \lambda$ unless there is some lowest value of μ , call it μ_ℓ , such that $J_- |\lambda\mu_\ell\rangle = 0$.

Now we use these conditions to show $\mu_h = -\mu_\ell$. Consider applying J_- to $J_+ |\lambda\mu_h\rangle = 0$. Note the identity:

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

Thus

$$J_- J_+ |\lambda\mu_h\rangle = (\lambda - \mu_h^2 - \hbar\mu_h) |\lambda\mu_h\rangle = 0.$$

Taking the matrix element with $\langle\lambda\mu_h|$ we find

$$\lambda - \mu_h^2 - \hbar\mu_h = 0.$$

Similarly,

$$J_+ J_- |\lambda\mu_\ell\rangle = (J^2 - J_z^2 + \hbar J_z) |\lambda\mu_\ell\rangle$$

leads to

$$\lambda - \mu_\ell^2 + \hbar\mu_\ell = 0.$$

Hence

$$\lambda = \underbrace{\mu_h(\mu_h + \hbar) = \mu_\ell(\mu_\ell - \hbar)}$$

Two solutions: $\mu_h = -\mu_\ell$

or $\mu_h = \mu_\ell - \hbar$ but this second solution must be rejected since μ_h was assumed to be larger than μ_ℓ .

Now we can conclude also that $\mu_h = \mu_\ell + n\hbar$ where n is some integer. This follows since, if we start from $|\lambda\mu_\ell\rangle$ and apply J_+ repeatedly, we obtain the sequence of eigenvectors:

$$\underbrace{|\lambda\mu_\ell\rangle}_{\mu_\ell}, \quad \underbrace{J_+|\lambda\mu_\ell\rangle}_{\mu_\ell+\hbar}, \quad \underbrace{J_+^2|\lambda\mu_\ell\rangle}_{\mu_\ell+2\hbar}, \quad \dots \quad \underbrace{J_+^n|\lambda\mu_\ell\rangle}_{\mu_\ell+n\hbar=\mu_h} = |\lambda\mu_n\rangle$$

Thus

$$\mu_h = -\mu_\ell = \mu_\ell + n\hbar$$

or

$$\underline{\mu_\ell = -\frac{n}{2}\hbar, \mu_h = +\frac{n}{2}\hbar}$$

where $n = 0, 1, 2, \dots$ is some integer (related to the value of λ).

For convenience, we write

$$\mu = m\hbar, \quad m = -j, -j+1, \dots, +j$$

where $j = \frac{n}{2}$, with $j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$

Then eigenvalues of J_z are $\underbrace{-j\hbar, (-j+1)\hbar, \dots, j\hbar}_{2j+1 \text{ different values}}$

Eigenvalues of J^2 are given by

$$\begin{aligned} \lambda &= \mu_h(\mu_h + \hbar) = \mu_\ell(\mu_\ell - \hbar) = j\hbar(j\hbar + \hbar) = -j\hbar(-j\hbar - \hbar) \\ \lambda &= j(j+1)\hbar^2 \end{aligned}$$

Also, it is convenient to label the eigenvectors by j, m rather than λ, μ , so

$$\begin{aligned} J^2 |jm\rangle &= j(j+1)\hbar^2 |jm\rangle \\ j_z |jm\rangle &= m\hbar |jm\rangle. \end{aligned}$$

Comments

We derived the above eigenvalues using only the commutation property and the Hermitian property. We find that both integer and half-integer values of j and m are allowed.

Actually, we have solved a much more general problem than that posed by the orbital angular momentum of a particle. Thus, for several particles in the same central force field, the total angular momentum,

$$\sum_n \underline{L}^{(n)},$$

also satisfies these relations, even if the particles interact with each other. Spin angular momenta likewise satisfy these relations.

For orbital angular momentum, $\underline{L} = \underline{q} \times \underline{p}$ must require, in addition, that the system returns to its original state under a rotation by 2π . Such a rotation takes $\underline{p} \rightarrow \underline{p}$ and $\underline{q} \rightarrow \underline{q}$ so $\underline{q} \times \underline{p} \rightarrow \underline{q} \times \underline{p}$ and hence the eigenvectors of L^2 and L_z must be unchanged:

$$e^{-i2\pi J_z/\hbar} |jm\rangle = e^{-i2\pi m} |jm\rangle$$

$e^{-i2\pi m} = +1$ if m is integer and hence integer eigenvalues are acceptable for L^2 , L_z . Half-integer values give $e^{-i2\pi m} = -1$ and hence are *not* acceptable for *orbital angular momentum*.

Half-integers do apply for *spin* angular momenta, which are not constructed from any $\underline{q} \times \underline{p}$ and thus can take on both integer and half-integer eigenvalues. This illustrates the power of operator derivation. A more general case would not have been included if we had used wave mechanical methods and representations by differential operators.

We have shown that, *for a fixed j value*,

$$J_+ |jm\rangle = a_m |j, m+1\rangle \quad \text{and} \quad J_- |jm\rangle = b_m |j, m-1\rangle,$$

where a_m and b_m are constants, possibly complex numbers. The proportionality constants are simply related to each other, since

$$\begin{aligned} a_m &= \langle j, m+1 | J_+ | jm \rangle = \left\langle jm \left| \underbrace{J_+^\dagger}_{J_-} \right| j, m+1 \right\rangle^* = \left(\int \psi_{jm}^* \underbrace{J_- \psi_{j, m+1}}_{b_{m+1} \psi_{j, m}} d\tau \right)^* \\ &= b_{m+1}^* \end{aligned}$$

Now, to evaluate a_m , consider the identity

$$J_- J_+ = J^2 - J_z^2 - \hbar J_z.$$

Apply this to $|jm\rangle$, then you have

$$\begin{aligned} J_- J_+ |jm\rangle &= a_m J_- |j, m+1\rangle = a_m b_{m+1} |jm\rangle = |a_m|^2 |jm\rangle \\ J^2 - J_z^2 - \hbar J_z |jm\rangle &= (j(j+1) - m^2 - m)\hbar^2 |jm\rangle. \end{aligned}$$

Hence

$$a_m = \underbrace{[j(j+1) - m(m+1)]^{1/2} \hbar e^{i\phi m}}_{(j-m)(j+m+1)} \leftarrow \text{another common way of writing it,}$$

where $e^{i\phi m}$ is an arbitrary phase factor. The usual convention is to take $\phi = 0$; this fixes the relative phases of the vectors $|jm\rangle$ having different values of m but the same j .

The only non-vanishing matrix elements of J_+ and J_- are:

$$\langle j, m+1 | J_+ | jm \rangle = \langle j, m | J_- | j, m+1 \rangle = [j(j+1) - m(m+1)]^{1/2} \hbar$$

↑
always the lower times the
higher of the two m -values in
the matrix element

Or you can write this alternatively as

$$\begin{aligned} \langle j', m' | J_+ | jm \rangle &= [j(j+1) - m(m+1)]^{1/2} \hbar \delta_{j',j} \delta_{m',m+1} \\ \langle j', m' | J_- | jm \rangle &= [j(j+1) - m(m-1)]^{1/2} \hbar \delta_{j',j} \delta_{m',m-1} \end{aligned}$$

List of non-zero elements:

$$\begin{aligned}
 jm|J^2|jm &= j(j+1)\hbar^2 && \text{"add the bigger } m \text{ to } j \text{ and} \\
 \langle jm|J_z|jm\rangle &= m\hbar && \text{subtract the smaller"} \\
 \langle j, m \pm 1|J_{\pm}|jm\rangle &= [j(j+1) - m(m \pm 1)]^{1/2}\hbar = \overbrace{[(j \pm m + 1)(j \mp m)]}^{1/2}\hbar \\
 J_x &= \frac{1}{2}(J_+ + J_-), \quad J_y = \frac{1}{2i}(J_+ - J_-) \\
 \langle j, m \pm 1|J_x|jm\rangle &= \frac{1}{2}[j(j+1) - m(m \pm 1)]^{1/2}\hbar \\
 \langle j, m \pm 1|J_y|jm\rangle &= \pm \frac{1}{2i}[j(j+1) - m(m \pm 1)]^{1/2}\hbar
 \end{aligned}$$

We can summarize elements of J_x, J_y, J_z by:

$$\begin{aligned}
 jm|J_z|jm &= \hat{z}m\hbar \\
 j, m \pm 1|J_x|jm &= (\hat{x} \pm i\hat{y})\frac{1}{2}[j(j+1) - m(m \pm 1)]^{1/2}\hbar.
 \end{aligned}$$

Comment

Thus we have found all matrix elements of J with eigenvectors $|jm\rangle$ of J^2, J_z . These eigenvectors and their properties are important, since any time we have a system of particles isolated in free space, their total angular momentum J^2, J_z commutes with the total Hamiltonian, no matter what kind of forces hold the system together (central or not). That is, the total angular momentum of an isolated system is a constant of the motion in quantum mechanics, just as in classical mechanics.

Hence it is important to be able to take matrix elements of other operators in the angular momentum states which characterize an isolated system.

Examples

$$j = 0 : \quad J_+ = (0) \quad J_- = (0) \quad J_z = (0) \quad J^2 = (0)$$

$$j = \frac{1}{2} : J_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad J_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad J_z = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} \quad J^2 = \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{3}{4} \end{pmatrix}$$

$j = 1$:

$$J_+ = \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \quad J_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$J_- = \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix} \quad J^2 = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

$j = \frac{3}{2}$:

$$J_+ = \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad J_z = \begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}$$

$$J_- = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix} \quad J^2 = \begin{pmatrix} \frac{15}{4} & 0 & 0 & 0 \\ 0 & \frac{15}{4} & 0 & 0 \\ 0 & 0 & \frac{15}{4} & 0 \\ 0 & 0 & 0 & \frac{15}{4} \end{pmatrix}$$

MOMENTA AS DISPLACEMENT OPERATORS:

Geometrical Meaning of Commutation Rules

Linear Momentum

Let $|x_1\rangle$ be an eigenvector of the position operator X with eigenvalue x_1 , i.e.

$$X |x_1\rangle = x_1 |x_1\rangle.$$

Consider the new state vector defined by $e^{-iap_x/\hbar} |x_1\rangle$; we might ask whether it is also an eigenvector of X . To find out, evaluate

$$X (e^{-iap_x/\hbar} |x_1\rangle) = e^{-iap_x/\hbar} \underbrace{(X |x_1\rangle)}_{x_1 |x_1\rangle} + \underbrace{[X, e^{-iap_x/\hbar}] |x_1\rangle}$$

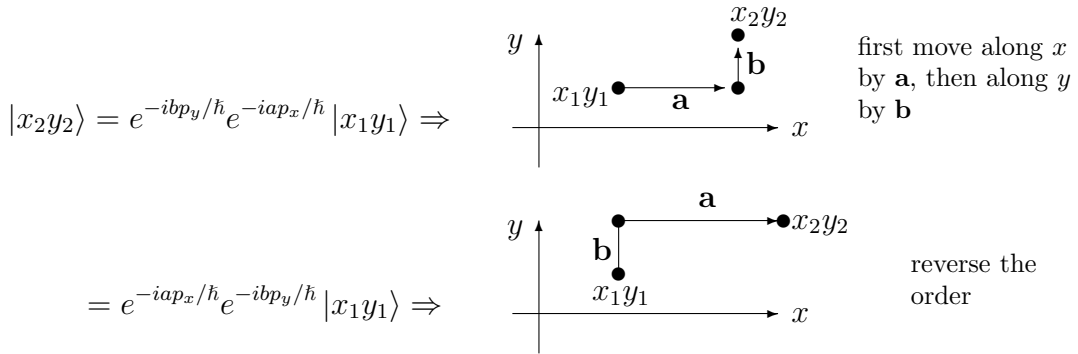
Now

$$\begin{aligned} [X, e^{-iap_x/\hbar}] &= i\hbar \frac{d}{dp_x} (e^{-iap_x/\hbar}) \\ &= ae^{-iap_x/\hbar} \end{aligned}$$

Thus

$$\begin{aligned} X (e^{-iap_x/\hbar} |x_1\rangle) &= e^{-iap_x/\hbar} (X + a) |x_1\rangle = e^{-iap_x/\hbar} (x_1 + a) |x_1\rangle \\ &= (x_1 + a) (e^{-iap_x/\hbar} |x_1\rangle). \end{aligned}$$

Hence $e^{-iap_x/\hbar} |x_1\rangle$ is indeed an eigenvector of X with eigenvalue $x_1 + a$ instead of x_1 . The unitary operator $e^{-iap_x/\hbar}$ formed from the linear momentum operator p_x acts as a *displacement operator* for x position coordinates. Similarly, p_y generates displacements of the y coordinate and p_z of the z coordinate. It is a geometrical fact that *linear displacements* of a point *commute*. For example:



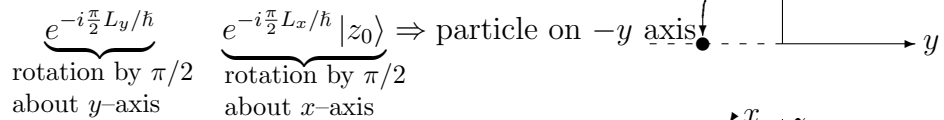
The same result is obtained by applying displacements in either order. This agrees with $[p_x, p_y] = 0$ (and $\{p_x, p_y\} = 0$).

Angular momentum

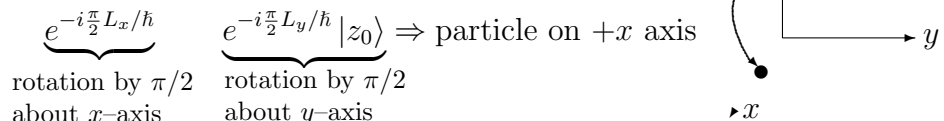
L_x, L_y, L_z operators generate *angular* displacements or *rotations*; e.g.,

$$e^{-i\phi L_x/\hbar}$$

gives a rotation by angle ϕ about the x -axis, etc. However, geometrical *rotations about different axes do not commute*. For example, consider a state representing a particle on the z -axis, $|z_0\rangle$. Now



But



The results of these two rotations taken in opposite order differ by a rotation about the z -axis. Thus, because the rotations about different axes don't commute, we must expect the angular momentum operators, which generate these rotations, *not* to commute with each other. Indeed,

$$[L_x, L_y] = i\hbar L_z$$

corresponds to the above example, in which the commutator of rotations about the x and y axes depends on a z -axis rotation.

Rotational Transformation Properties and Selection Rules

The various observables of a dynamical system can be classified according to their transformation properties under rotations. This is of great value in determining the matrix elements of the corresponding operators and, in particular, leads to selection rules which limit the number of non-zero matrix elements.

Under action of the rotation operator $U = e^{i\phi \cdot \mathcal{J}/\hbar}$ an operator O is transformed according to

$$O' = UOU^\dagger.$$

A *scalar* operator \mathcal{S} is one which is invariant to this transformation (e.g., the Hamiltonian of an isolated system). Hence, for a scalar operator

$$U\mathcal{S}U^\dagger = \mathcal{S}$$

or

$$U\mathcal{S} - \mathcal{S}U = 0 \quad \text{or} \quad [U, \mathcal{S}] = 0.$$

Thus, a scalar commutes with every rotation operator. Consider, in particular, an infinitesimal rotation $d\phi$, for which

$$U = 1 + \frac{i}{\hbar} d\phi \cdot \mathcal{J}.$$

Since the direction of $d\phi$ is arbitrary, \mathcal{S} must commute with each component of \mathcal{J} , or $[\mathcal{S}, \mathcal{J}] = 0$. As shown below, this property leads to the selection rules

$$\Delta j = 0, \quad \Delta m = 0$$

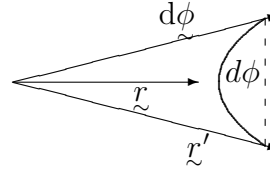
for the non-zero matrix elements of a scalar operator.

A *vector* operator \mathcal{V} is one with three components, V_x, V_y, V_z which transform under rotations like the coordinates of a point. For an infinitesimal rotation,

$$\mathcal{V}' = \left(1 + \frac{i}{\hbar} d\phi \cdot \mathcal{J}\right) \mathcal{V} \left(1 - \frac{i}{\hbar} d\phi \cdot \mathcal{J}\right).$$

Now note that if the position vector \tilde{r}' is obtained from \tilde{r} by rotation through a small angle $d\phi$ about an axis in the direction of the vector $d\phi$, we have, to first order in $d\phi$,

$$\tilde{r}' = \tilde{r} + d\phi \times \tilde{r}$$



and so

$$\tilde{V}' = \tilde{V} + d\phi \times \tilde{V}.$$

Hence, if terms in $(d\phi)^2$ are neglected, we obtain

$$d\phi \times \tilde{V} = \frac{i}{\hbar} \left[(d\phi \cdot \tilde{J}) \tilde{V} - \tilde{V} (d\phi \cdot \tilde{J}) \right].$$

Since $d\phi$ is arbitrary, this relation gives the commutator of \tilde{V} with any component of \tilde{J} . Thus, if $d\phi = \varepsilon \hat{z}$ is a rotation about the z -axis, we find

$$\varepsilon(\hat{z} \times \tilde{V}) = \varepsilon \frac{i}{\hbar} [J_z \tilde{V} - \tilde{V} J_z]$$

or

$$\begin{aligned} [J_z, \tilde{V}] &= -i\hbar(\hat{z} \times \tilde{V}) & \text{or} & & [J_z, V_x] &= -i\hbar(-V_y) = i\hbar V_y \\ & & & & [J_z, V_y] &= -i\hbar(-V_x) = -i\hbar V_x \\ & & & & [J_z, V_z] &= 0 \end{aligned}$$

etc.

In this way we obtain a set of nine commutation rules:

$$\begin{array}{lll} [J_x, V_x] = 0 & [J_y, V_x] = -i\hbar V_z & [J_z, V_x] = -i\hbar V_y \\ [J_x, V_y] = i\hbar V_z & [J_y, V_y] = 0 & [J_z, V_y] = -i\hbar V_x \\ [J_x, V_z] = -i\hbar V_y & [J_y, V_z] = i\hbar V_x & [J_z, V_z] = 0 \end{array}$$

The selection rules for non-zero matrix elements of a vector operator, i.e. an operator which satisfies the above rules (e.g., position \tilde{r} , linear momentum \tilde{p} , the angular momentum \tilde{J} itself) are shown below to be given by

$$\Delta j = 0 \text{ and } \pm 1 \text{ for all components of } \tilde{V}$$

with

$$\begin{aligned}\Delta m &= 0 \text{ for } V_z \\ \Delta m &= \pm 1 \text{ for } V_{\pm} = V_x \pm iV_y.\end{aligned}$$

Scalar Operators, \mathbf{S}^1

Defined by $[\mathcal{L}, \mathcal{J}] = 0$, for all three components of \mathcal{J} . Corollary is $[S, J^2] = 0$ and $[S, J_z] = 0$. If we take the matrix elements, we have

$$\begin{aligned}j'm' \langle [S, J^2] | jm \rangle &= 0 \\ &= j'm' \langle SJ^2 - J^2S | jm \rangle \\ &= \hbar^2 \langle j'm' | Sj(j+1) - j'(j'+1)S | jm \rangle \\ &= \hbar^2 [j(j+1) - j'(j'+1)] \langle j'm' | S | jm \rangle.\end{aligned}$$

Also,

$$\begin{aligned}\langle j'm' | [S, J_z] | jm \rangle &= 0 \\ &= \langle j'm' | SJ_z - J_zS | jm \rangle \\ &= \hbar \langle j'm' | Sm - m'S | jm \rangle \\ &= \hbar(m - m') \langle j'm' | S | jm \rangle.\end{aligned}$$

Therefore, $\langle j'm' | S | jm \rangle$ must vanish unless $j = j'$ and $m' = m'$. “Selection rules” for non-zero elements are: $\Delta j = 0$ and $\Delta m = 0$.

Let $s_{jm} \equiv \langle jm | S | jm \rangle$ denote the non-vanishing element. Since this is the only non-zero matrix element, $|jm\rangle$ is an eigenvector of S , i.e. $S|jm\rangle = s_{jm}|jm\rangle$. Now we can show that the eigenvalues of the scalar operator S don't depend on m . Since S commutes with $J_{\pm} = J_x \pm iJ_y$, we have

$$S(J_+ |jm\rangle) = J_+ S |jm\rangle = s_{jm} (J_+ |jm\rangle).$$

But $J_+ |jm\rangle$ is proportional to $|j, m+1\rangle$ and still has some eigenvalue s_{jm} of S . We could continue this with $J_+^2 \rightarrow m+2, \dots$ and with $J_- \rightarrow m-1$,

¹These notes were prepared by Professor Dudley Herschbach of Harvard University

$J_-^2 \rightarrow m-2$, etc., and would get the same eigenvalue s_{jm} of S for all m states of a given j . Hence we would obtain

$$\langle j'm'|S|jm\rangle = \langle j||S||j\rangle \delta_{jj'}\delta_{mm'}$$

where $\langle j||S||j\rangle$ is called a *reduced* matrix element, a number that does *not* depend on m .

The above equation only describes the properties of S which are associated with its scalar character. In general, the states of the system will depend upon other quantum numbers in addition to j and m . If these are denoted collectively by α , the scalar operator need not be diagonal in α , so the general statement becomes

$$\langle \alpha'j'm'|S|\alpha jm\rangle = \langle \alpha'j||S||\alpha j\rangle \delta_{jj'}\delta_{mm'}$$

for

$$[S, \underline{J}] = 0.$$

Vector Operators, \underline{V}

Definition: A *vector* operator \underline{V} with respect to the angular momentum \underline{J} is any set of three operators V_x, V_y, V_z that satisfy the following commutation rules:

$$\begin{aligned} [J_i, V_j] &= i\hbar \sum_k \varepsilon_{ijk} V_k & \varepsilon_{ijk} &= 1, ijk \text{ cyclic} \\ & & &= -1, ijk \text{ anti-cyclic} \\ & & &= 0, \text{ any two subscripts the same} \end{aligned}$$

This is shorthand for

$$\begin{array}{lll} [J_x, V_x] = 0 & [J_y, V_x] = -i\hbar V_z & [J_z, V_x] = i\hbar V_y \\ [J_x, V_y] = i\hbar V_z & [J_y, V_y] = 0 & [J_z, V_y] = -i\hbar V_x \\ [J_x, V_z] = -i\hbar V_y & [J_y, V_z] = i\hbar V_x & [J_z, V_z] = 0. \end{array}$$

It is convenient to use

$$V_{\pm} = V_x \pm iV_y \quad V_x = \frac{1}{2}(V_+ + V_-); \quad V_y = \frac{1}{2i}(V_+ - V_-).$$

Selection Rules for m

Consider the commutators involving J_z , take matrix elements of the commutators:

$$\text{a) } [J_z, V_z] = 0$$

$$\langle j'm' | J_z V_z - V_z J_z | jm \rangle = \langle j'm' | m' \hbar V_z - V_z m \hbar | jm \rangle = \hbar(m' - m) \langle j'm' | V_z | jm \rangle$$

$$\text{Thus } \langle j'm' | V_z | jm \rangle = 0 \text{ unless } m' = m, \underline{\Delta m = 0}$$

$$\text{b) } [J_z, V_+] = [J_z, V_x + iV_y] = i\hbar V_y + i(-i\hbar V_x) = \hbar V_+$$

$$\langle j'm' | J_z V_+ - V_+ J_z | jm \rangle = \hbar \langle j'm' | V_+ | jm \rangle.$$

or

$$\hbar(m' - m - 1) \langle j'm' | V_+ | jm \rangle = 0$$

$$\langle j'm' | V_+ | jm \rangle = 0 \text{ unless } m' - m = +1, \underline{\Delta m = +1}$$

$$\text{c) Similarly, } [J_z, V_-] = -\hbar V_- \text{ and}$$

$$\langle j'm' | V_- | jm \rangle = 0 \text{ unless } m' - m = -1, \underline{\Delta m = -1}$$

Selection Rules for j

To find the selection rules for j , we want to examine commutators of \underline{V} with \underline{J}^2 . For this, some vector identities are useful. First we show

$$(1) \quad \underline{J} \times \underline{V} + \underline{V} \times \underline{J} = 2i\hbar \underline{V}.$$

This relation is another way to define a vector operator. It states that, because of the non-commuting algebra of quantum mechanics, $\underline{J} \times \underline{V} \neq -\underline{V} \times \underline{J}$ as would hold for ordinary vectors.

0.0.1 Proof:

$$\begin{aligned}
(\underline{J} \times \underline{V} + \underline{V} \times \underline{J})_i &= \sum_{j,k} (\varepsilon_{ijk} J_j V_k + \varepsilon_{ijk} V_j J_k) \quad \text{re-label via } j \leftrightarrow k \\
&= \sum_{j,k} \varepsilon_{ijk} (J_j V_k - V_k J_j) \quad \text{Then use } \varepsilon_{ijk} = -\varepsilon_{ikj} \\
&= \sum_{j,k} \varepsilon_{ijk} [J_j, V_k] = i\hbar \sum_{jkl} \varepsilon_{ijk} \varepsilon_{jkl} V_l \quad \text{using the definition} \\
& \quad \text{of a vector operator}
\end{aligned}$$

Note $\varepsilon_{ijk}\varepsilon_{jkl} = \varepsilon_{ijk}\varepsilon_{ljk}$ as a cyclic permutation of subscripts leaves ε_{ijk} unchanged.

Then

$$\sum_{j,k} \varepsilon_{ijk}\varepsilon_{ljk} = 2\delta_{il} \quad \begin{array}{l} \text{factor 2 appears because both odd-odd} \\ \text{and even-even permutations give a} \\ \text{contribution} \end{array}$$

So

$$(\underline{J} \times \underline{V} + \underline{V} \times \underline{J})_i = 2i\hbar \sum_{\ell} \delta_{i\ell} V_{\ell} = 2i\hbar V_i \quad \text{Q.E.D.}$$

Now we show

$$(2) \quad [\underline{J}^2, \underline{V}] = i\hbar(\underline{V} \times \underline{J} - \underline{J} \times \underline{V}).$$

Proof:

$$\begin{aligned}
[J^2, V_j] &= \sum_i [J_i^2, V_j] \\
&= \sum_i \{J_i [J_i, V_j] + [J_i, V_j] J_i\} \\
[J^2, V_j] &= i\hbar \sum_{i,k} \left\{ J_i \underbrace{\varepsilon_{ijk}} V_k + \underbrace{\varepsilon_{ijk}} V_k J_i \right\} \\
&= i\hbar(-\underline{J} \times \underline{V} + \underline{V} \times \underline{J})_j \quad \text{Q.E.D.}
\end{aligned}$$

It is convenient to define the operator

$$\underline{K} \equiv \frac{1}{2}(\underline{V} \times \underline{J} - \underline{J} \times \underline{V}).$$

This is Hermitian (since \underline{V} and \underline{J} are) and is a vector operator if \underline{V} is.

Then Equation (2) states

$$[\underline{J}^2, \underline{V}] = 2i\hbar\underline{K}. \quad (1)$$

However, we can't yet use this commutator to get selection rules on \underline{V} , since the matrix elements of the commutator \underline{K} would seem to bear no simple relation to those of \underline{V} . We will find that selection rules can be obtained from an identity involving the double commutator,

$$(3) \quad [\underline{J}^2, [\underline{J}^2, \underline{V}]] = 2\hbar^2\{\underline{J}^2\underline{V} - 2(\underline{J} \cdot \underline{V})\underline{J} + \underline{V}\underline{J}^2\}.$$

This can be proven by examining further the properties of \underline{K} .

$$[\underline{J}^2, [\underline{J}^2, \underline{V}]] = 2i\hbar[\underline{J}^2, \underline{K}].$$

Since \underline{K} is a vector operator, we have from (2) that

$$[\underline{J}^2, \underline{K}] = i\hbar(\underline{K} \times \underline{J} - \underline{J} \times \underline{K}).$$

Also, from Equation (1) we have

$$\underline{J} \times \underline{K} + \underline{K} \times \underline{J} = 2i\hbar\underline{K}.$$

Hence

$$\begin{aligned} \underline{J} \times \underline{K} - \underline{K} \times \underline{J} &= \underline{J} \times \underline{K} - (2i\hbar\underline{K} - \underline{J} \times \underline{K}) \\ &= 2\underline{J} \times \underline{K} - 2i\hbar\underline{K}. \end{aligned}$$

Also, from equation (1)

$$\underline{K} \equiv \frac{1}{2}(\underline{V} \times \underline{J} - \underline{J} \times \underline{V}) = \underline{V} \times \underline{J} - i\hbar\underline{V}.$$

Thus,

$$\begin{aligned} \underline{J} \times \underline{K} &= J \times (V \times \underline{J}) - i\hbar(\underline{J} \times V) \\ (\underline{J} \times \underline{K})_i &= \underbrace{\sum_{j,k} \varepsilon_{ijk} J_j (V \times \underline{J})_k - i\hbar(\underline{J} \times V)_i}_{\sum_{jklm} \varepsilon_{ijk} J_j \varepsilon_{klm} V_l J_m} \end{aligned}$$

shift to $\varepsilon_{lmk} = \varepsilon_{klm}$ since cyclic permutation of subscripts leaves ε unchanged

$$\begin{aligned} \sum_{jlm} |(\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}) J_j V_l J_m &= \sum_j (J_j V_i J_j - J_j V_j J_i) \\ &= \sum_j (J_j J_j V_i - J_j [J_j, V_i] - J_j V_j J_i) \\ &= J^2 V_i - \underbrace{\sum_{j\ell} J_j i\hbar \varepsilon_{j\ell} V_\ell}_{\uparrow} - (\underline{J} - V) J_i \end{aligned}$$

replace by $-\varepsilon_{ij\ell}$, a non-cyclic permutation

$$+ i\hbar \sum_{j\ell} J_j \varepsilon_{ij\ell} V_\ell = i\hbar(\underline{J} \times V)_i.$$

So we find

$$(\underline{J} \times \underline{K})_i = \underline{J}^2 V_i - (\underline{J} \cdot V) J_i + \cancel{i\hbar(\underline{J} \times V)_i} - \cancel{i\hbar(\underline{J} \times V)_i}$$

or

$$\underline{J} \times \underline{K} = \underline{J}^2 V - (\underline{J} \cdot V) \underline{J}.$$

Now we can use these results to simplify the double commutator,

$$\begin{aligned} [\underline{J}^2, [\underline{J}, V]] &= 2i\hbar[\underline{J}^2, \underline{K}] = (2i\hbar)(i\hbar)(-1)(2\underline{J} \times \underline{K} - 2i\hbar\underline{K}) \\ &= 2\hbar^2(2\underline{J} \times \underline{K} - 2i\hbar\underline{K}) \\ &= 2\hbar^2\{2\underline{J}^2 V - 2(\underline{J} \cdot V)\underline{J} - \underbrace{[\underline{J}^2, V]}\} \end{aligned}$$

$$J^2 \underline{V} - \underline{V} J^2$$

and finally,

$$[\underline{J}, [J^2, \underline{V}]] = 2\hbar^2 \{J^2 \underline{V} - 2(\underline{J} \cdot \underline{V}) \underline{J} + \underline{V} J^2\} \quad \text{Q.E.D.}$$

Now we can obtain selection rules by taking matrix elements of this relation. Consider two cases:

Case I: Elements diagonal in j : Wigner-Eckart Theorem

$$jm' | [J^2, A] | jm \rangle = \langle jm' | j(j+1)A - Aj(j+1) | jm \rangle = 0$$

for any operator A . Thus,

$$jm' | [J^2, [J^2, \underline{V}]] | jm \rangle = 0 = 2\hbar^2 \langle jm' | J^2 \underline{V} - 2(\underline{J} \cdot \underline{V}) \underline{J} + \underline{V} J^2 | jm \rangle$$

or

$$\begin{aligned} \hbar^2 j(j+1) \langle jm' | \underline{V} | jm \rangle - \underbrace{\langle jm' | (\underline{J} \cdot \underline{V}) \underline{J} | jm \rangle}_{=} &= 0 \\ &= \sum_{j'' m''} \langle jm' | (\underline{J} \cdot \underline{V}) | j'' m'' \rangle \langle j'' m'' | \underline{J} | jm \rangle . \end{aligned}$$

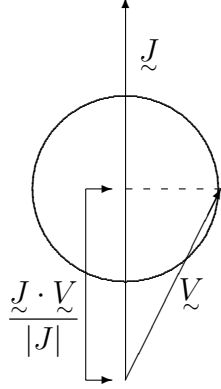
The operator $(\underline{J} \cdot \underline{V})$ is a *scalar* with respect to \underline{J} and therefore diagonal in both m and j , so that $j'' = j$ and $m'' = m'$, and its matrix elements are independent of m . Hence we find

$$\boxed{\langle jm' | \underline{V} | jm \rangle = \frac{j \langle \underline{J} \cdot \underline{V} | j \rangle}{\hbar^2 j(j+1)} \langle jm' | \underline{V} | jm \rangle}$$

This is the Wigner-Eckart theorem for a vector operator.

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$$jm'|\underline{V}|jm\rangle = \frac{j|\underline{J} \cdot \underline{V}|j}{j(j+1)\hbar^2} jm'|\underline{J}|jm\rangle$$



Suppose \underline{V} precesses around \underline{J} . The time averaged value of the component normal to \underline{J} is zero. The time average of \underline{V} is therefore parallel to \underline{J} and has magnitude

$$\frac{\underline{J} \cdot \underline{V}}{|\underline{J}|}.$$

Hence, on this model, the average is

$$\underline{V} = \frac{\underline{J} \cdot \underline{V}}{J^2} \underline{J} = \frac{(\underline{J} \cdot \underline{V})}{|\underline{J}|} \frac{\underline{J}}{|\underline{J}|}$$

The theorem is very useful, as it states that, for any vector operator \underline{V} , the matrix elements diagonal in j are simply proportional to the corresponding matrix elements of \underline{J} itself. The proportionality constant, $c_0(j) = j|(\underline{J} \cdot \underline{V})|j\rangle / (\hbar j(j+1))$ is the same for all m -states. Therefore, we have via the Wigner-Eckart Theorem:

$$\langle j, m+1 | V_+ | jm \rangle = c_0(j) [j(j+1) - m(m+1)]^{1/2}$$

$$\langle jm | V_z | jm \rangle = c_0(j) m$$

$$\langle j, m-1 | V_- | jm \rangle = c_0(j) [j(j+1) - m(m-1)]^{1/2}$$

with $c_0(j) = \langle \alpha' j || V || \alpha j \rangle$ a reduced matrix element. In particular, we note that all matrix elements of \underline{V} between $j=0$ states vanish.

Case II: Elements non-diagonal in j

Now consider $j' \neq j$, again take matrix elements of Equation (3). LHS gives

$$\begin{aligned} j'm'[[J^2, [J^2, V]]|jm\rangle &= j'm'|J^2(J^2V - VJ^2) - (J^2V - VJ^2)J^2|jm\rangle \\ &= \{j'^2(j'+1)^2 - 2j(j+1)j(j+1) + j^2(j+1)^2\} \langle j'm'|V|jm\rangle. \end{aligned}$$

RHS gives

$$2\hbar^2 \left\langle j'm' | J^2 \underline{V} - \underbrace{2(\underline{J} \cdot \underline{V}) \underline{J}} + \underline{V} J^2 | jm \right\rangle = 2\hbar^2 \{j'(j'+1) + j(j+1)\} j'm' | \underline{V} | jm$$

drops out as $j'm' | \underline{J} | jm = 0$, because $j' \neq j$.

Equating LHS = RHS and rearranging gives

$$\{(j' - j)^2 - 1\} \underbrace{\{(j' + 1 + 1)^2 - 1\}} j'm' | \underline{V} | jm = 0$$

This factor > 0 since $j' \neq j$ and $j' \geq 0, j \geq 0$

Therefore

$$j'm' | \underline{V} | jm = 0$$

unless $(j' - j)^2 - 1 = 0$ or $j' = j \pm 1$.

The *complete selection rules* for any vector operator thus are:

$$j'm' | \underline{V} | jm = 0 \text{ unless}$$

$$j' = j \neq 0 \quad \text{or} \quad j' = j \pm 1$$

and, for any j', j

$$m' = m \text{ or } m' = m \pm 1.$$

We have already found (page 19) the matrix element for $j' = j$. Now we will do $j' = j + 1$.

$$\begin{aligned} \text{Consider } [J_+, V_+] &= [J_x + iJ_y, V_x + iV_y] \\ &= [J_x, V_x] + i[J_x, V_y] + i[J_y, V_x] - [J_y, V_y] \\ &\quad \downarrow \quad \downarrow \quad \downarrow \quad \downarrow \\ &= 0 \quad i\hbar V_z \quad -i\hbar V_z \quad 0 \\ &= 0. \end{aligned}$$

Take matrix element and use $\langle j, m+1 | J_+ | j, m \rangle = \hbar[j(j+1) - m(m+1)]^{1/2}$
 $= \hbar[(j+m+1)(j-1)]^{1/2}$

$$\begin{aligned} 0 &= \langle j+1, m+1 | (J_+ V_+ - V_+ J_+) | j, m-1 \rangle \\ &= \langle j+1, m+1 | J_+ | j+1, m \rangle \langle j+1, m | V_+ | j, m-1 \rangle \\ &\quad - \langle j+1, m+1 | V_+ | jm \rangle \langle jm | J_+ | j, m-1 \rangle \end{aligned}$$

where we use the $\Delta m = +1$ selection rule for V_+ and J_+ .

This provides a recurrence relation for the matrix elements.

$$\begin{aligned} \langle j+1, m+1 | J_+ | j+1, m \rangle \langle j+1, m | V_+ | j, m-1 \rangle &= \langle j+1, m+1 | V_+ | jm \rangle \\ &\quad \times \langle jm | J_+ | j, m-1 \rangle \\ \hbar[(j-m+1)(j+m+2)]^{1/2} &\quad \hbar[(j-m+1)(j+m)]^{1/2} \end{aligned}$$

So

$$\frac{\langle j+1, m | V_+ | j, m-1 \rangle}{(j+m)^{1/2}} = \frac{\langle j+1, m+1 | V_+ | j, m \rangle}{(j+m+2)^{1/2}}.$$

This takes on a simple pattern if we divide both sides by $(j+m+1)^{1/2}$:

$$\begin{aligned} -c_+(j, m) &\equiv \frac{\langle j+1, m | V_+ | j, m-1 \rangle}{[(j+m+1)(j+m)]^{1/2}} = \frac{\langle j+1, m+1 | V_+ | j, m \rangle}{[(j+m+2)(j+m+1)]^{1/2}} \\ &= -c_+(j, m+1). \end{aligned}$$

Since m was arbitrary, $c_+(j, m) = c_+(j, m+1) = c_+(j, \text{any other } m)$ so the ratio $c_+(j)$ must be independent of m . The m -independence of the matrix element is therefore given by

$$\langle j+1, m+1 | V_+ | j, m \rangle = -c_+(j)[(j+m+2)(j+m+1)]^{1/2},$$

with $c_+(j) = \alpha', j+1 \| \mathcal{V} \| \alpha, j$ a reduced matrix element that depends on the detailed nature of \mathcal{V} , not merely on its vector character. However, it can be evaluated if the matrix element of \mathcal{V} can be evaluated for any single m value, e.g., $m = j$ or $m = 0$, for which the evaluation is often simpler than in the general case.

Now determine the $j' = j + 1$ elements of V_Z using the above result for V_+ . Start with

$$-2\hbar V_Z = [J_-, V_+] \quad \text{which expresses } V_Z \text{ in terms of } J_- \text{ and } V_+, \\ \text{whose matrix elements we now know.}$$

$$\begin{aligned} -2\hbar \langle j+1, m | V_Z | j, m \rangle &= \langle j+1, m | J_- | j+1, m+1 \rangle \langle j+1, m+1 | V_+ | j, m \rangle \\ &\quad - \langle j+1, m | V_+ | j, m-1 \rangle \langle j, m-1 | J_- | j, m \rangle \\ &= \hbar [(j+m+2)(j-m+1)]^{1/2} (-c_+(j)) [(j+m+2)(j+m+1)]^{1/2} \\ &\quad - \hbar (-c_+(j)) [(j+m+1)(j+m)]^{1/2} [(j+m)(j-m+1)]^{1/2} \\ &= -\hbar c_+(j) [(j+m+2) - (j+m)] [(j+m+1)(j-m+1)]^{1/2} \\ &= -2\hbar c_+(j) [(j+m+1)(j-m+1)]^{1/2} \end{aligned}$$

Thus,

$$\langle j+1, m | V_Z | j, m \rangle = c_+(j) [(j+m+1)(j-m+1)]^{1/2}.$$

Similarly, from

$$\hbar V_- = [J_-, V_Z]$$

we find

$$\langle j+1, m-1 | V_- | j, m \rangle = c_+(j) [(j-m+2)(j-m+1)]^{1/2}.$$

Results for $j' = j - 1$ are derived in analogous fashion and involve a third reduced matrix element, $c_-(j) = \langle \alpha', j-1 | V_- | \alpha, j \rangle$. Hence the m -dependence of a scalar or vector operator follows from its scalar or vector character *only*. Classification of operators by their transformation properties under rotation can be extended to tensors of any rank. In each case the form of the matrix elements is determined except for factors that depend on α and j .

SUMMARY: Non-zero Matrix Elements of a Vector Operator, \hat{V}

$$\begin{aligned} \Delta j = +1 \quad \langle j+1, m \pm 1 | V_{\pm} | jm \rangle &= \mp c_+(j) [(j \pm m + 2)(j \pm m + 1)]^{1/2} \\ \langle j+1, m | V_Z | jm \rangle &= c_+(j) [(j+m+1)(j-m+1)]^{1/2} \end{aligned}$$

$$\begin{aligned} \Delta j = 0 \quad \langle j, m \pm 1 | V_{\pm} | jm \rangle &= c_0(j) [(j \pm m + 1)(j \mp m)]^{1/2} \\ \langle jm | V_Z | jm \rangle &= c_0(j) m \end{aligned}$$

$$\begin{aligned} \Delta j = -1 \quad \langle j-1, m \pm 1 | V_{\pm} | jm \rangle &= \pm c_-(j) [(j \mp m)(j \mp m - 1)]^{1/2} \\ \langle j-1, m | V_Z | jm \rangle &= c_-(j) [(j-m)(j+m)]^{1/2} \end{aligned}$$

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