

# Quantum theory of angular momentum

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Time: Friday, 13:00 –14:30

Place: Freihaus, **Sem.R. DA grün 06B**

(exception date 18 Nov.: **Sem.R. DA grün 06A**)

Lecture notes will appear at:

<http://atomchip.org/theory/>

## Recommended literature

1. Varshalovich, Moskalev, Khersonsky „Quantum theory of angular momentum“

other specialized literature:

2. Edmonds „Angular momentum in quantum mechanics“
3. Fano & Racah „Irreducible tensorial sets“
4. Wigner „Group theory“

some material in standard courses:

5. Landau & Lifshitz „Quantum Mechanics“
6. Akhiezer & Berestetsky „Quantum Electrodynamics“

...and in any other q.m.-textbook where you can find it...

# 0. Notation

Vector

Vector component

Unit vector

$$\mathbf{A} = \sum_{\alpha} A^{\alpha} \mathbf{e}_{\alpha} = \sum_{\alpha} A_{\alpha} \mathbf{e}^{\alpha}$$

Lower index – covariant

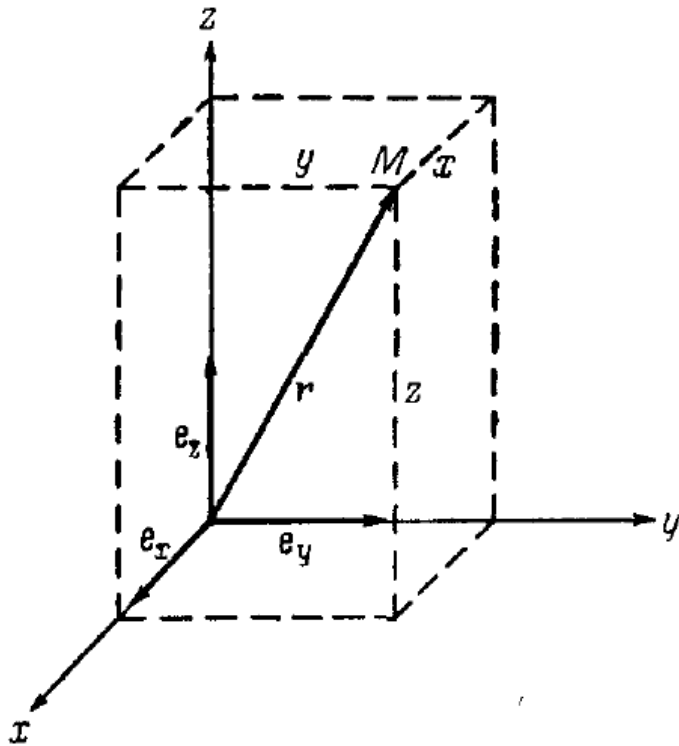
Upper index – contravariant

$$\mathbf{e}_{\mu} \mathbf{e}^{\nu} = \delta_{\mu\nu}$$

$$A_{\alpha} = \mathbf{A} \cdot \mathbf{e}_{\alpha}, \quad A^{\alpha} = \mathbf{A} \cdot \mathbf{e}^{\alpha}$$

# Co-ordinate system

## Cartesian

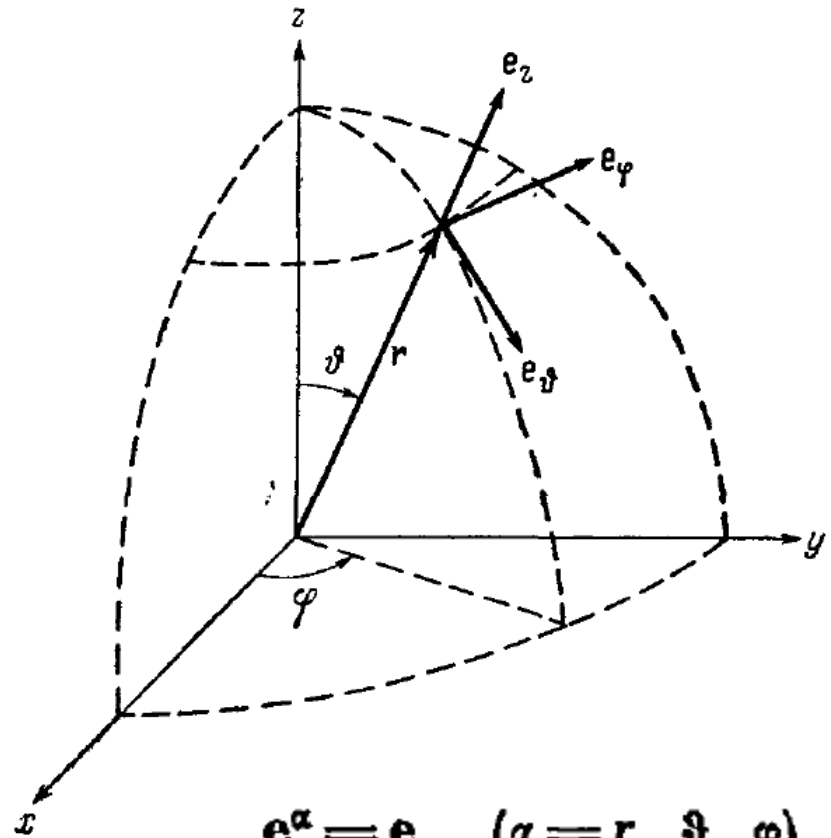


$$\mathbf{e}^i = \mathbf{e}_i$$

$$[\mathbf{e}_i \times \mathbf{e}_k] = \varepsilon_{ikl} \mathbf{e}_l, \quad (i, k, l = x, y, z)$$

Levi-Civita tensor

## spherical



$$\mathbf{e}^\alpha = \mathbf{e}_\alpha \quad (\alpha = r, \vartheta, \varphi)$$

$$[\mathbf{e}_r \times \mathbf{e}_\vartheta] = \mathbf{e}_\varphi, \quad [\mathbf{e}_\vartheta \times \mathbf{e}_\varphi] = \mathbf{e}_r,$$

$$[\mathbf{e}_\varphi \times \mathbf{e}_r] = \mathbf{e}_\vartheta$$

## Cyclic coordinates

$$x_{+1} = -\frac{1}{\sqrt{2}}(x + iy) = -\frac{1}{\sqrt{2}}r \sin \vartheta e^{i\varphi},$$

Covariant

$$x_0 = z = r \cos \vartheta,$$

$$x_{-1} = \frac{1}{\sqrt{2}}(x - iy) = \frac{1}{\sqrt{2}}r \sin \vartheta e^{-i\varphi}.$$

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$$x^{+1} = -\frac{1}{\sqrt{2}}(x - iy) = -\frac{1}{\sqrt{2}}r \sin \vartheta e^{-i\varphi},$$

Contravariant

$$x^0 = z = r \cos \vartheta,$$

$$x^{-1} = \frac{1}{\sqrt{2}}(x + iy) = \frac{1}{\sqrt{2}}r \sin \vartheta e^{i\varphi}.$$

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$$\begin{aligned} x^\mu &= (-1)^\mu x_{-\mu}, & x_\mu &= (-1)^\mu x^{-\mu}, & (\mu = \pm 1, 0) \\ x^\mu &= x_\mu^*, & x_\mu &= x^{\mu*}, \end{aligned}$$

Cyclic unit vectors

$$\mathbf{e}_{+1} = -\frac{1}{\sqrt{2}} (\mathbf{e}_x + i\mathbf{e}_y),$$

Covariant

$$\begin{aligned}\mathbf{e}_0 &= \mathbf{e}_z, \\ \mathbf{e}_{-1} &= \frac{1}{\sqrt{2}} (\mathbf{e}_x - i\mathbf{e}_y).\end{aligned}$$

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Contravariant

$$\begin{aligned}\mathbf{e}^{+1} &= -\frac{1}{\sqrt{2}} (\mathbf{e}_x - i\mathbf{e}_y), \\ \mathbf{e}^0 &= \mathbf{e}_z, \\ \mathbf{e}^{-1} &= \frac{1}{\sqrt{2}} (\mathbf{e}_x + i\mathbf{e}_y).\end{aligned}$$

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$$\mathbf{e}^\mu = (-1)^\mu \mathbf{e}_{-\mu}, \quad \mathbf{e}_\mu = (-1)^\mu \mathbf{e}^{-\mu}, \quad (\mu = \pm 1, 0).$$

$$\mathbf{e}^\mu = \mathbf{e}_\mu^*, \quad \mathbf{e}_\mu = \mathbf{e}^{\mu*},$$

$$\mathbf{e}_\mu \mathbf{e}^\nu = \mathbf{e}_\mu \mathbf{e}_\nu^* = \delta_{\mu\nu}$$

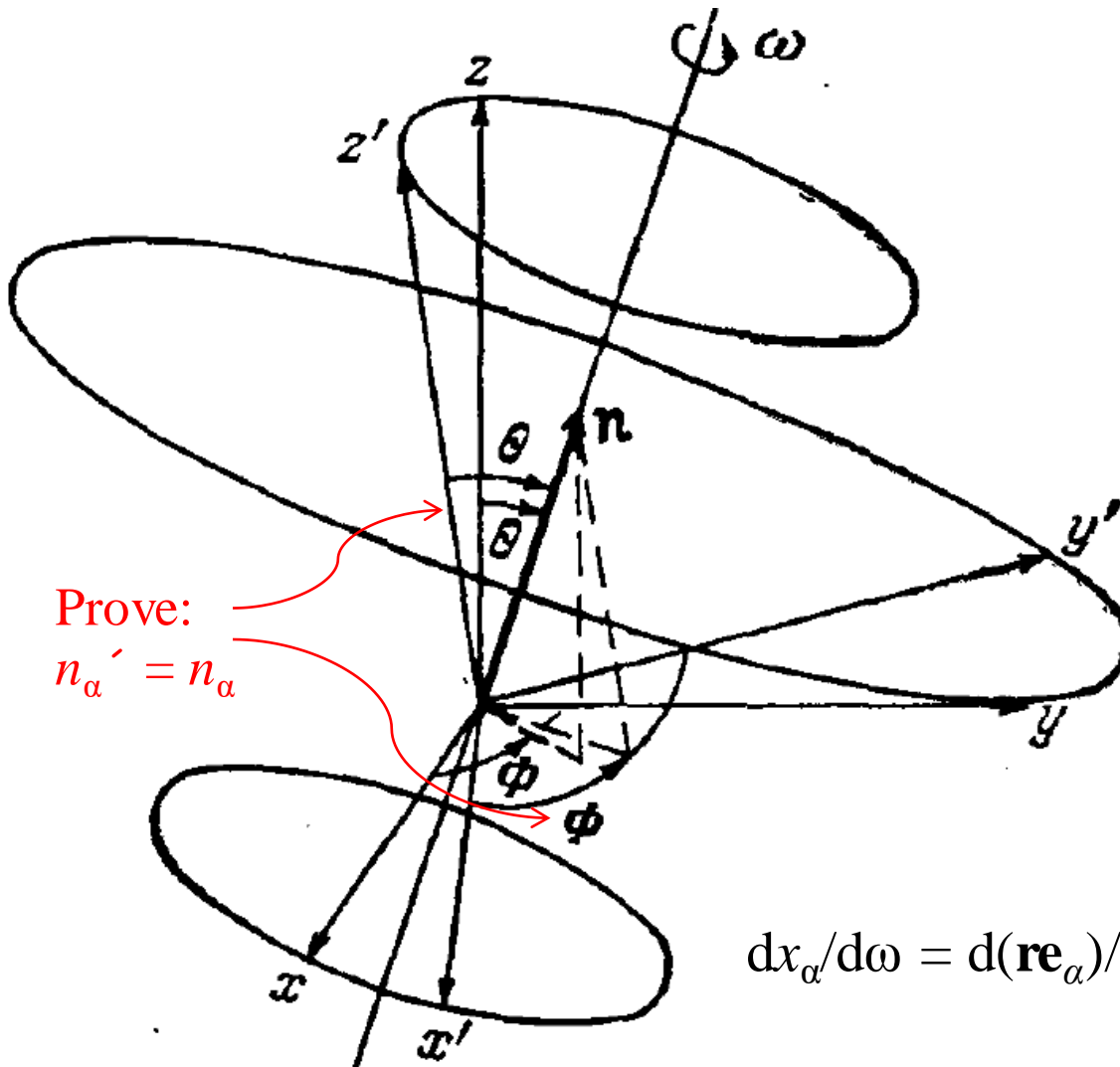
# I. Rotation operation

An isolated quantum system in a 3D space ( $r =$  all variables)

$$\begin{aligned}\hat{H}\Psi_{\epsilon\pi\alpha jm}(r) &= \epsilon\Psi_{\epsilon\pi\alpha jm}(r), && \text{Energy} \\ \hat{P}_r\Psi_{\epsilon\pi\alpha jm}(r) &= \pi\Psi_{\epsilon\pi\alpha jm}(r), && \text{Parity} \\ \mathbf{J}^2\Psi_{\epsilon\pi\alpha jm}(r) &= j(j+1)\Psi_{\epsilon\pi\alpha jm}(r), && \text{Square of the total angular momentum} \\ \hat{J}_z\Psi_{\epsilon\pi\alpha jm}(r) &= m\Psi_{\epsilon\pi\alpha jm}(r). && \text{Ang.momentum projection to } z \text{ axis}\end{aligned}$$

How is the wave function transformed under a rotation of the co-ordinate system?

We consider **passive** rotations: the physical system remains at rest, but the coordinate system is rotated.



The rotation is given by

- 1) the rotation angle  $\omega$ ;
- 2) the direction of the rotation axis: unit vector  $\mathbf{n} = \mathbf{e}_x \sin \Theta \cos \Phi + \mathbf{e}_y \sin \Theta \sin \Phi + \mathbf{e}_z \cos \Theta$

Consider  $\omega$  as a parameter of a continuous transformation from  $S$  to  $S'$ :

$$d\mathbf{e}_\alpha/d\omega = [\mathbf{n} \times \mathbf{e}_\alpha]$$

$$dx'_\alpha/d\omega = d(\mathbf{r}\mathbf{e}_\alpha)/d\omega = \mathbf{r} d\mathbf{e}_\alpha/d\omega = \mathbf{r} [\mathbf{n} \times \mathbf{e}_\alpha]$$



What we do (starting with a function of co-ordinates of one particles):

1. Make co-ordinate system rotation, calculate the new  $\mathbf{r}' = (x', y', z')$  as a function of  $\mathbf{r} = (x, y, z)$ ,  $\omega$ , and  $\mathbf{n}$ .
2. Choose an arbitrary (differentiable) function  $\Psi$ .
3. Find, which operator relates this function in the new coordinates to the same function in the old co-ordinates:

$$\Psi(\mathbf{r}') = \hat{D}(\omega, \mathbf{n})\Psi(\mathbf{r})$$

Again, consider  $\mathbf{r}$  as a value parametrized by the variable  $\omega$  and finally reaching  $\mathbf{r}'$ . Then

$$\frac{d}{d\omega} \Psi(\mathbf{r}) = \frac{\partial \hat{D}(\omega, \mathbf{n})}{\partial \omega} \Psi(\mathbf{r})$$

$$\begin{aligned} \frac{d}{d\omega} \Psi(\mathbf{r}) &= \frac{d\mathbf{r}}{d\omega} \nabla \Psi(\mathbf{r}) = \sum_{\alpha=x,y,z} \frac{dx_{\alpha}}{d\omega} \frac{\partial}{\partial x_{\alpha}} \Psi(\mathbf{r}) = \\ &= \sum_{\alpha=x,y,z} \mathbf{r}[\mathbf{n} \times \mathbf{e}_{\alpha}] \frac{\partial}{\partial x_{\alpha}} \Psi(\mathbf{r}) = \mathbf{r}[\mathbf{n} \times \nabla] \Psi(\mathbf{r}) = -\mathbf{n}[\mathbf{r} \times \nabla] \Psi(\mathbf{r}) \end{aligned}$$

Recall the orbital momentum operator  $\hat{\mathbf{L}} = -i[\mathbf{r} \times \nabla]$ .

Then one can see that

$$\frac{\partial \hat{D}(\omega, \mathbf{n})}{\partial \omega} = -i \mathbf{n} \hat{\mathbf{L}}, \quad \hat{D}(0, \mathbf{n}) = 1$$

$$\hat{D}(\omega, \mathbf{n}) = \exp(-i \omega \mathbf{n} \hat{\mathbf{L}})$$

The latter equation holds in a case of a function of co-ordinates of  $N$  particles.

In that case  $\hat{\mathbf{L}} = \sum_{j=1}^N \hat{\mathbf{L}}^{(j)}$  is the total orbital momentum.

$$[\hat{\mathbf{L}}, \hat{\mathbf{L}}^2] = 0$$

Therefore an eigenfunction of the operator  $\hat{\mathbf{L}}^2$  with the eigenvalue  $= L(L+1)$  is transformed after a rotation into a linear combination of the eigenfunctions with the same total orbital momentum  $L$ .

There are in total  $2L+1$  different functions for a given  $L$ , characterized by

$$L_z = -L, -L+1, \dots, L-1, L.$$

How to **interpret** and **extend** this observation?

# Rotations as a group

Definition of a group.

Group is a set  $G$ . An operation  $\bullet$  (the group law) is defined so that

1. If  $a \in G$  and  $b \in G$  then  $a \bullet b \in G$ .
2. Associativity:  $\forall \{a, b, c\} \subset G$  we have  $(a \bullet b) \bullet c = a \bullet (b \bullet c)$ .
3. Identity element:  $\exists e \in G$  such that  $\forall a \in G$  we have  $e \bullet a = a \bullet e = a$ .

In fact, the identity element is always unique.

4. Inverse element:  $\forall a \in G$  an element  $a^{-1} \in G$  exists, such that  
$$a^{-1} \bullet a = a \bullet a^{-1} = e.$$

The rotations satisfy all these requirements, the operation  $\bullet$  being a subsequent performance of two rotations.

Every group can be characterized by its irreducible representations.

An irreducible representation is a set of objects where a linear combination is defined and

- (i) that is mapped to itself under action of any element of the group (*representation*), but
- (ii) it is impossible to make (by constructing linear combinations) its subset, which also would be a representation (*irreducibility*).

The irreducible representations (IRs) of the rotation group have dimensions 1, 2, 3, 4, ... , each dimension appearing only once.

Odd-dimensional IRs can be associated with a system characterized by an integer angular momentum (realizable by the orbital momentum).

The even-dimensional IRs can be associated with a system with a half-integer angular momentum (realizable by the spin).

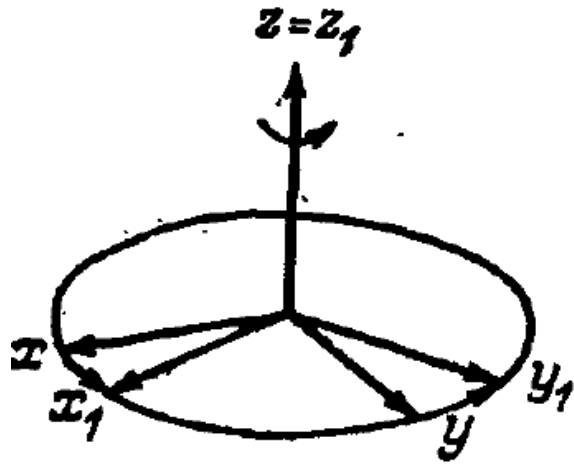
Then in a general case  $\hat{D}(\omega, \mathbf{n}) = \exp(-i \omega \mathbf{n} \hat{\mathbf{J}})$  ,

where  $\hat{\mathbf{J}}$  is the angular momentum operator (without concretization of its orbital, spin or composite nature).

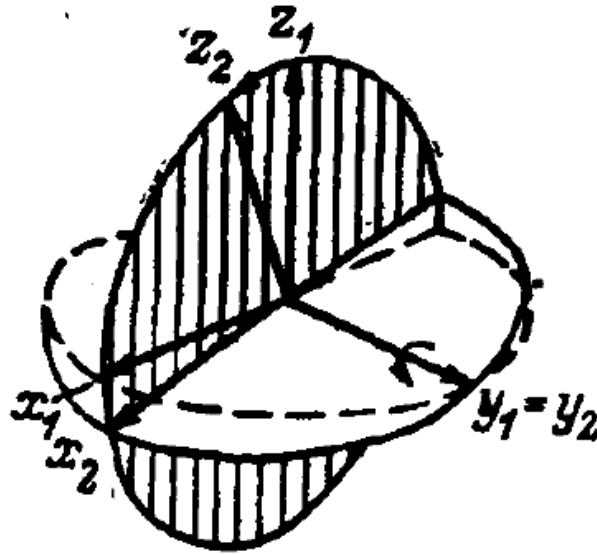
# Euler angles

Alternatively, a rotation may be defined with three Euler angles.

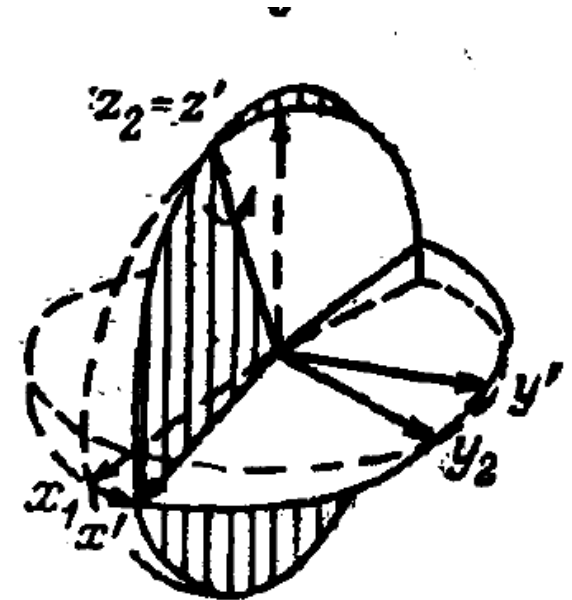
Scheme A:



(i) Rotation around  $z$  by  $\alpha$  ( $0 \leq \alpha < 2\pi$ ).



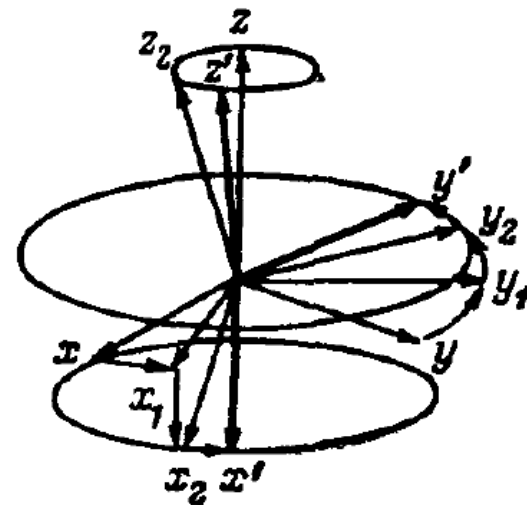
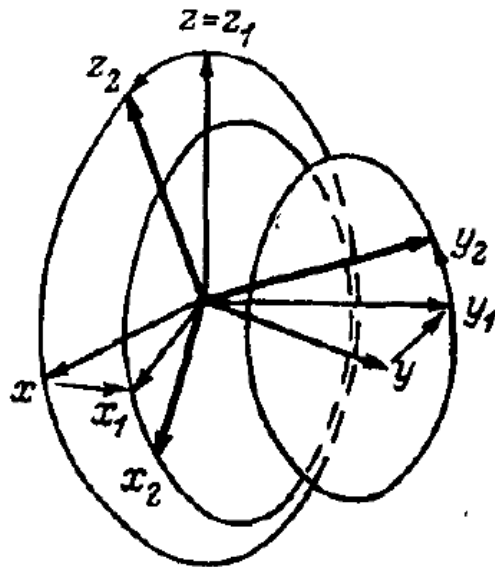
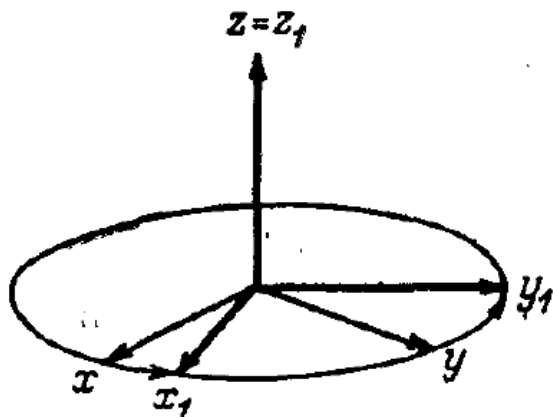
(ii) Rotation around *new*  $y_1$  by  $\beta$  ( $0 \leq \beta < \pi$ ).



(iii) Rotation around *final*  $z_2 = z'$  by  $\gamma$  ( $0 \leq \gamma < 2\pi$ ).

Scheme B (equivalent to A, angles are the same).

Three rotations around the *old* axes.



(i) Rotation around  $z$  by  $\gamma$  ( $0 \leq \gamma < 2\pi$ ).

(ii) Rotation around  $y$  by  $\beta$  ( $0 \leq \beta < \pi$ ).

(iii) Rotation around  $z$  by  $\alpha$  ( $0 \leq \alpha < 2\pi$ ).

The same rotation is achieved also with  $\alpha' = \alpha + \frac{\pi}{2}$ ,  $\beta' = \beta$ ,  $\gamma' = \gamma - \frac{\pi}{2}$

The polar angles of an arbitrary directions in  $S' \{x', y', z'\}$  and  $S \{x, y, z\}$  are related as

$$\cos \vartheta' = \cos \vartheta \cos \beta + \sin \vartheta \sin \beta \cos (\varphi - \alpha)$$

$$\text{ctg} (\varphi' + \gamma) = \text{ctg} (\varphi - \alpha) \cos \beta - \frac{\text{ctg} \vartheta \sin \beta}{\sin (\varphi - \alpha)}$$

From now on, we put Euler angles as the arguments of the rotation operator  $\hat{D}(\alpha, \beta, \gamma)$ . A function in the new coordinate and an operator are expressed as

$$\Psi' = \hat{D}(\alpha, \beta, \gamma) \Psi, \quad O' = \hat{D}(\alpha, \beta, \gamma) O [\hat{D}(\alpha, \beta, \gamma)]^{-1}$$

$$\hat{D}(\alpha, \beta, \gamma) = e^{-i\gamma \hat{J}_{z'}} e^{-i\beta \hat{J}_{y_1}} e^{-i\alpha \hat{J}_z} \quad \text{(scheme A)}$$

(3) Rotation around *final*  
 $z_2 = z'$  by  $\gamma$  ( $0 \leq \gamma < 2\pi$ ).

(2) Rotation around *new*  
 $y_1$  by  $\beta$  ( $0 \leq \beta < \pi$ ).

(1) Rotation around  $z$  by  
 $\alpha$  ( $0 \leq \alpha < 2\pi$ ).

*Try to prove their  
 equivalence!*

or, equivalently, 
$$\hat{D}(\alpha, \beta, \gamma) = e^{-i\alpha \hat{J}_z} e^{-i\beta \hat{J}_y} e^{-i\gamma \hat{J}_z}$$

(scheme B)

(3) Rotation around  $z$   
 by  $\alpha$  ( $0 \leq \alpha < 2\pi$ ).

(2) Rotation around  $y$   
 by  $\beta$  ( $0 \leq \beta < \pi$ ).

(1) Rotation around  $z$   
 by  $\gamma$  ( $0 \leq \gamma < 2\pi$ ).

Unitarity:

$$\hat{D}^\dagger(\alpha, \beta, \gamma) = [\hat{D}(\alpha, \beta, \gamma)]^{-1} = \hat{D}(\pi - \gamma, \beta, -\pi - \alpha) = \hat{D}(-\gamma, -\beta, -\alpha)$$

Wigner  $D$ -function (definition)

$$\langle J'M' | \hat{D}(\alpha, \beta, \gamma) | JM \rangle = \delta_{JJ'} D_{M'M}^J(\alpha, \beta, \gamma)$$

We denote by  $X$  the angular (orbital & spin) variables of a system.

$$\begin{aligned} \langle X' | JM' \rangle &= \langle X | \hat{D}(\alpha, \beta, \gamma) | JM' \rangle = \langle X | \sum_{J''} \sum_M | J'' M \rangle \langle J'' M | \hat{D}(\alpha, \beta, \gamma) | JM' \rangle = \\ &= \sum_M \langle X | JM \rangle \langle JM | \hat{D}(\alpha, \beta, \gamma) | JM' \rangle \sum_M \langle X | JM \rangle D_{MM'}^J(\alpha, \beta, \gamma) \end{aligned}$$

$$\Psi_{JM'}(\vartheta', \varphi', \sigma') = \sum_{M=-J}^J \Psi_{JM}(\vartheta, \varphi, \sigma) D_{MM'}^J(\alpha, \beta, \gamma)$$

$$[\hat{D}^{-1}(\alpha, \beta, \gamma)]_{MM'}^J = D_{M'M}^{J*}(\alpha, \beta, \gamma)$$

$$\Psi_{JM}(\vartheta, \varphi, \sigma) = \sum_{M'=-J}^J D_{M'M}^{J*}(\alpha, \beta, \gamma) \Psi_{JM'}(\vartheta', \varphi', \sigma')$$