Quantum theory of angular momentum

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Time: Tuesday, 16:00 –18:00
Place: Atominstitute, Library (1st floor)
(exception date Mon. 29 Apr.)

Lecture notes:
http://atomchip.org/theory/lectures/

Recommended literature

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

   other specialized literature:

2. Edmomds „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 $_{\text{index}}$ – covariant

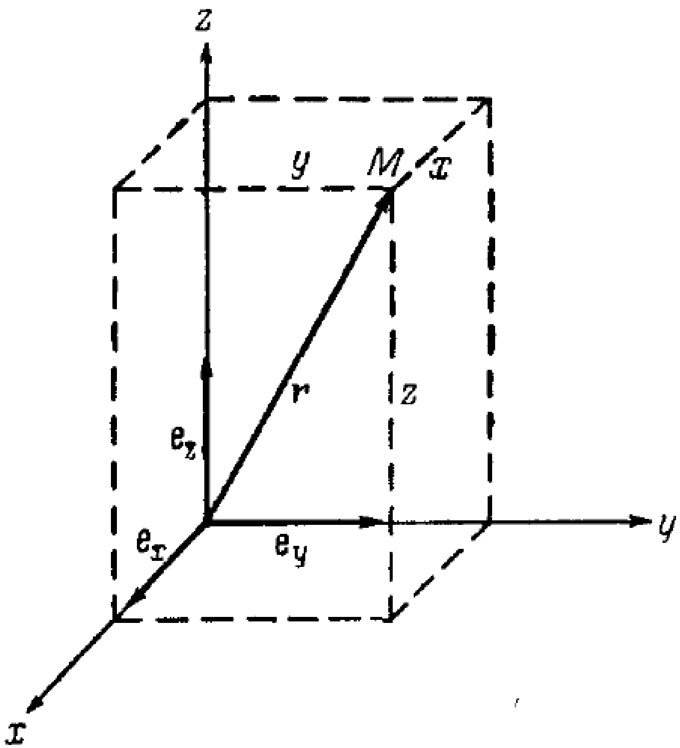
Upper $^{\text{index}}$ – contravariant

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

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

Co-ordinate system

Cartesian

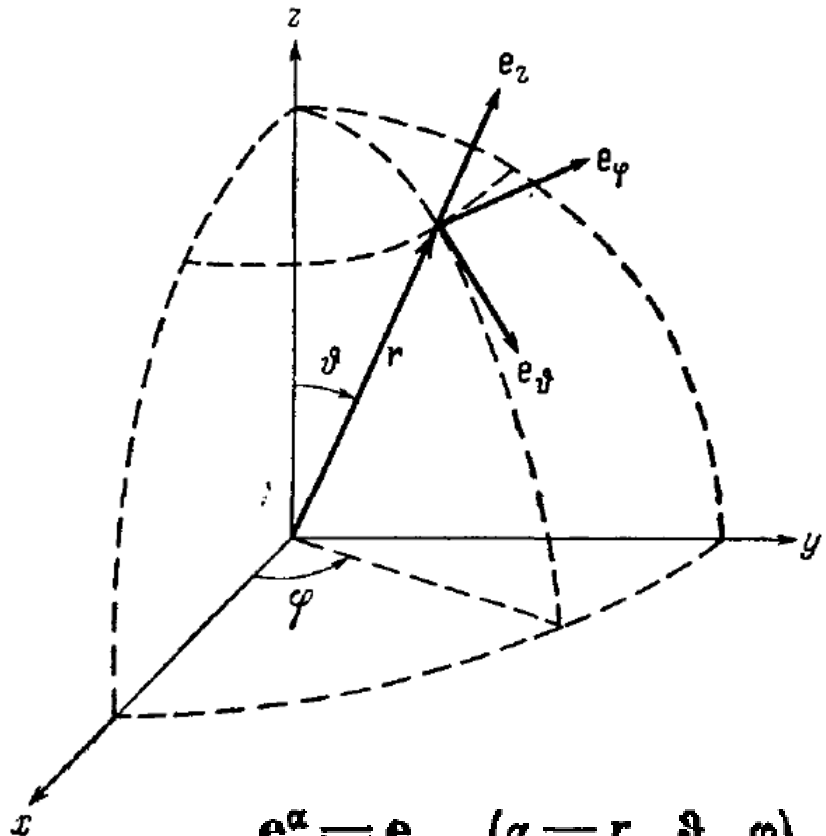


$$\mathbf{e}^i = \mathbf{e}_i$$

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

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

Covariant

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

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

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

Contravariant

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

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

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

$$x^\mu = (-1)^\mu x_{-\mu}, \quad x_\mu = (-1)^\mu x^{-\mu}, \qquad (\mu = \pm 1,\ 0)$$
$$x^\mu = x_\mu^*, \quad x_\mu = x^{\mu *},$$

Cyclic unit vectors

Covariant

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

$$\mathbf{e}_0 = \mathbf{e}_z,$$

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

Contravariant

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

$$\mathbf{e}^0 = \mathbf{e}_z,$$

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

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

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

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

I. Rotation operation

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

$$\hat{H}\Psi_{\varepsilon\pi\alpha jm}(r) = \varepsilon\Psi_{\varepsilon\pi\alpha jm}(r),$$ Energy

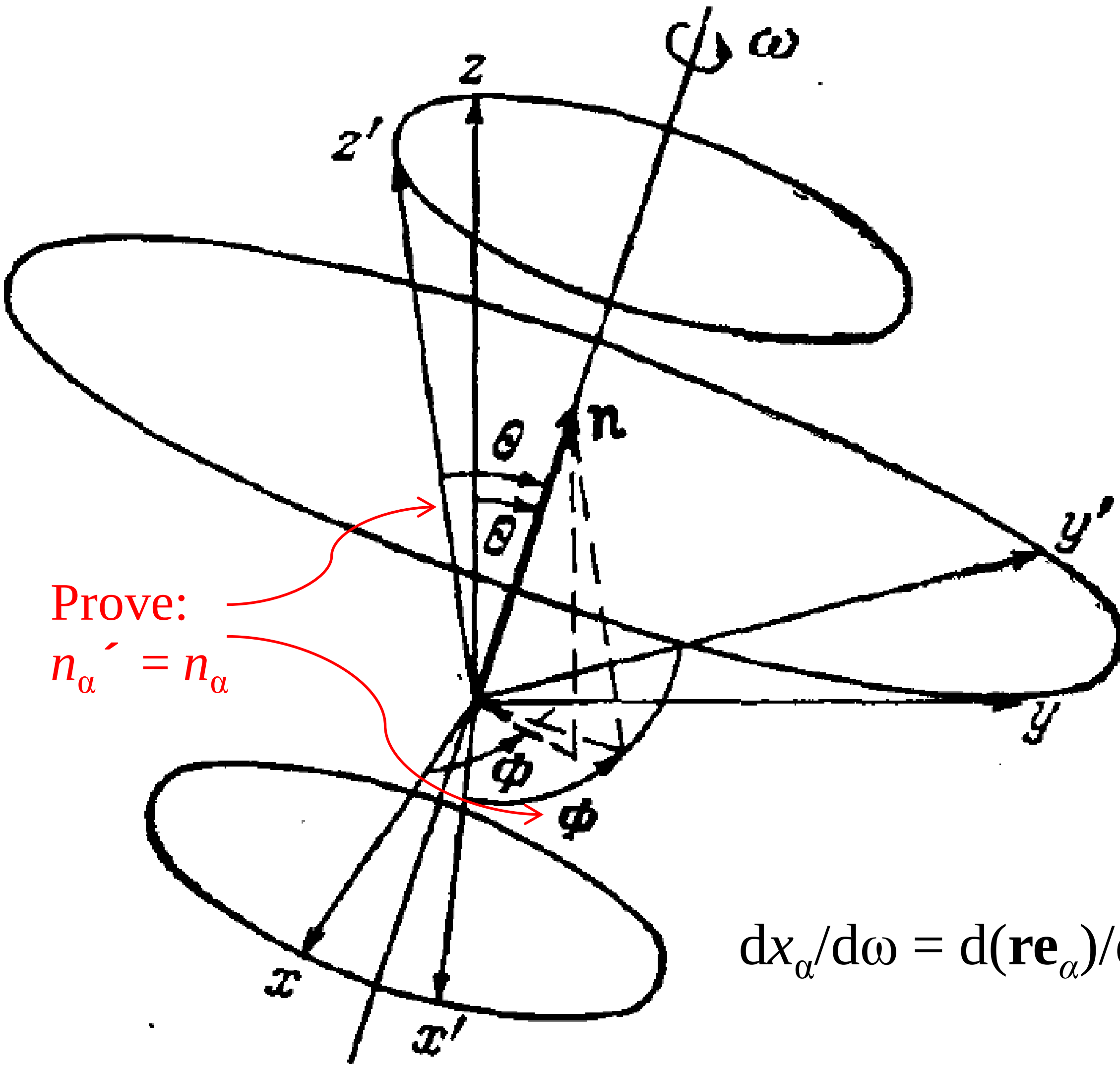
$$\hat{P}_r\Psi_{\varepsilon\pi\alpha jm}(r) = \pi\Psi_{\varepsilon\pi\alpha jm}(r),$$ Parity

$$\mathbf{J}^2\Psi_{\varepsilon\pi\alpha jm}(r) = j(j+1)\Psi_{\varepsilon\pi\alpha jm}(r),$$ Square of the total angular momentum

$$\hat{J}_z\Psi_{\varepsilon\pi\alpha jm}(r) = m\Psi_{\varepsilon\pi\alpha jm}(r).$$ Ang.momentum projection to z axis

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 co-ordinate system is rotated.



Prove:
$n_\alpha{}' = n_\alpha$

The rotation is given by

1) the rotation angle ω;
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 ω 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 a single particle):

1. Perform co-ordinate system rotation, calculate the new **r**´ = (x´ , y´ , z´) as a function of **r** = (x, y, z), ω, and **n**.
2. Choose an arbitrary (differentiable) function Ψ.
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 **r** as a value parametrized by the variable ω and finally reaching **r**´ . Then

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

$$\frac{d}{d\omega}\Psi(\mathbf{r}) = \frac{d\mathbf{r}}{d\omega}\nabla\Psi(\mathbf{r}) = \sum_{\alpha=x,y,z}\frac{dx_\alpha}{d\omega}\frac{\partial}{\partial x_\alpha}\Psi(\mathbf{r}) =$$

$$= \sum_{\alpha=x,y,z}\mathbf{r}[\mathbf{n}\times\mathbf{e}_\alpha]\frac{\partial}{\partial x_\alpha}\Psi(\mathbf{r}) = \mathbf{r}[\mathbf{n}\times\nabla]\Psi(\mathbf{r}) = -\mathbf{n}[\mathbf{r}\times\nabla]\Psi(\mathbf{r})$$

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

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

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

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
$L_Z = -L, -L+1, \ldots, L-1, L$.
How to interprete and extend this observation?

Rotations as a group

Definition of a group.

Group is a set $\mathcal{G}$. An operation • (the group law) is defined so that

1. If $a \in \mathcal{G}$ and $b \in \mathcal{G}$ then $a \bullet b \in \mathcal{G}$.
2. Associativity: $\forall \{a,b,c\} \subset \mathcal{G}$ we have $(a \bullet b) \bullet c = a \bullet (b \bullet c)$.
3. Identity element: $\exists e \in \mathcal{G}$ such that $\forall a \in \mathcal{G}$ we have $e \bullet a = a \bullet e = a$.
   In fact, the identity element is always unique.
4. Inverse element: $\forall a \in \mathcal{G}$ an element $a^{-1} \in \mathcal{G}$ exists, such that
   $a^{-1} \bullet a = a \bullet a^{-1} = e$.

The rotations satisfy all these requirements, the operation • 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.

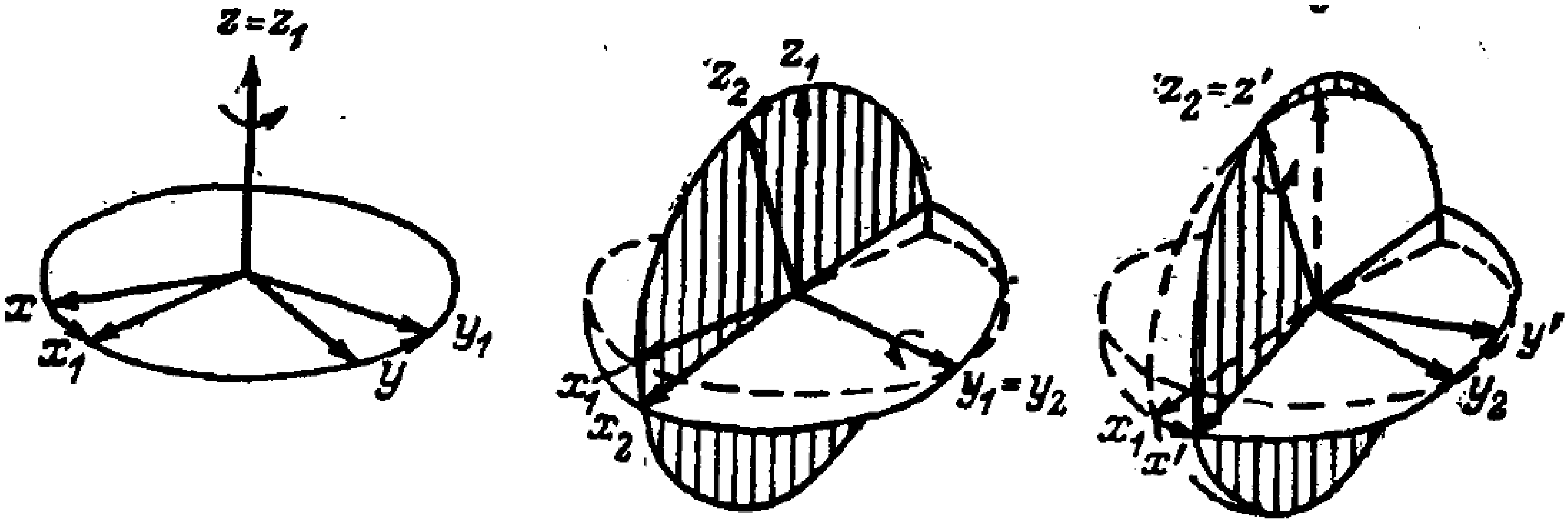
Odd-dimensional IRs can be associated with a system characterized by an integer angular momentum (realizable by the orbital momentum).
The even-dimensional IRs can be associated with a system with a half-integer angular momentum (realizable by the spin of a fermion).

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:

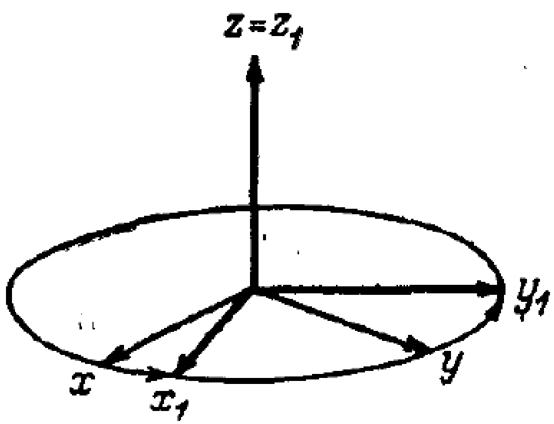


(i) Rotation around z by α ($0 \leq \alpha < 2\pi$).

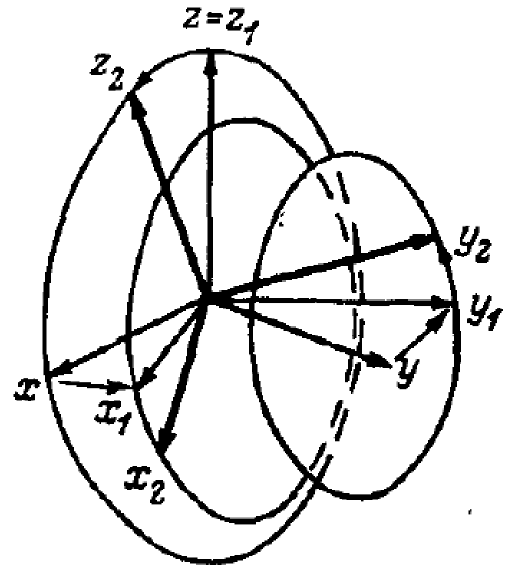
(ii) Rotation around ***new*** y_1 by β ($0 \leq \beta < \pi$).

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

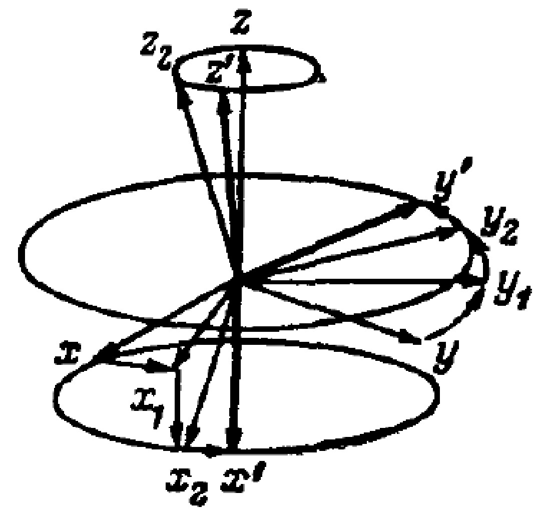
Scheme B (equivalent to A, angles are the same).
Three rotations around the ***old*** axes.



(i) Rotation around *z* by γ $(0 \le \gamma < 2\pi)$.



(ii) Rotation around *y* by β $(0 \le \beta < \pi)$.



(iii) Rotation around *z* by α $(0 \le \alpha < 2\pi)$.

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

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

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

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

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

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

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

(scheme A)

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

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

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

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 α ($0 \leq \alpha < 2\pi$).

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

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

Unitarity:

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

Wigner *D*-function (definition)

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

We denote by *Ω* the angular (orbital & spin) variables of a system.

$$\langle \Omega' | JM' \rangle = \langle \Omega | \hat{D}(\alpha,\beta,\gamma) | JM' \rangle = \langle \Omega | \sum_{J''} \sum_{M} | J''M \rangle \langle J''M | \hat{D}(\alpha,\beta,\gamma) | JM' \rangle =$$

$$= \sum_{M} \langle \Omega | JM \rangle \langle JM | \hat{D}(\alpha,\beta,\gamma) | JM' \rangle = \sum_{M} \langle \Omega | JM \rangle D^{J}_{MM'}(\alpha,\beta,\gamma)$$

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

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

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