4-2a Degrees of Freedom Associated with Spatial Rotations

Rotational motion in two dimensions (rotation about a fixed axis) has a very simple structure. The orientation is characterized by the azimuthal angle ϕ, and the state of motion by the eigenvalue M of the conjugate angular momentum. The associated rotational wave function is

$$\varphi_M(\phi) = (2\pi)^{-1/2} \exp\{iM\phi\} \tag{4-5}$$

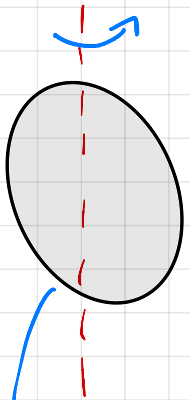
The orientation of a body in three-dimensional space involves three angular variables, such as the Euler angles, $\omega = \phi, \theta, \psi$ (see Fig. 1A-1, Vol. I, p. 76), and three quantum numbers are needed in order to specify the state of motion. The total angular momentum I and its component $M = I_z$ on a space-fixed axis provide two of these quantum numbers; the third may be obtained by considering the components of $\mathbf{I}$ with respect to an intrinsic (or body-fixed) coordinate system with orientation ω (see Sec. 1A-6a). The

→ 2D - rotation

rotation about a fixed axis

2D - rotation → $\boxed{\text{azimuthal angle } \phi}$ → orientation

→ $\boxed{M \to \text{eigenvalue of the conjugate angular momentum}}$ → state of motion



$$\varphi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{iM\phi}$$

$\omega \equiv$ orientation

3D - rotation

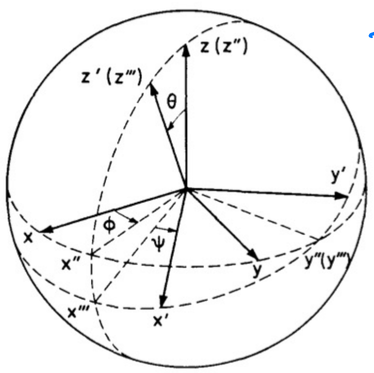


Figure 1A-1 Euler angles. The rotation from $\mathscr{K}(x, y, z)$ to $\mathscr{K}'(x', y', z')$ can be decomposed into three parts: a rotation by ϕ about the z axis to $\mathscr{K}''(x'', y'', z'')$, a rotation of θ about the new y axis (y'') to $\mathscr{K}'''(x''', y''', z''')$, and finally a rotation of ψ about the new z axis (z'''). It is seen that the Euler angles (ϕ, θ, ψ) are so defined that (θ, ϕ) are the polar angles of z' in $\mathscr{K}$, while (θ, $\pi - \psi$) are the polar angles of z in $\mathscr{K}'$. The Euler angles are, collectively, denoted by ω.

ORIENTATION

$\omega \to \phi, \theta, \psi$

3 angular variables (Euler)

STATE OF MOTION

3 quantum numbers

1 total angular momentum I

2 $M = I_z$: component on a space-fixed axis

3 System with orientation $\omega \to$ intrinsic c.s.
↳ component of I w.r.t ↑
I_3, K = component of I on body-fixed c.s

"c.s." ≡ coordinate system

1A-2 Coupling of Angular Momenta

If two components in the system have angular momenta j_1 and j_2, the coupling of these two components may produce states with resultant angular momentum

$$J = |j_1 - j_2|, |j_1 - j_2| + 1, \ldots, j_1 + j_2 \tag{1A-5}$$

The coupled states JM can be written in the form

$$|(j_1 j_2)JM\rangle \equiv |j_1 j_2\rangle_{(j_1 j_2)JM} = \sum_{m_1 m_2} |j_1 m_1, j_2 m_2\rangle \langle j_1 m_1 j_2 m_2 | JM\rangle \tag{1A-6}$$

$I_{1,2,3} \to$ – body-fixed
– scalars
– independent of the orientation

$I_{x,y,z} \to$ – space-fixed

I_{123} commute with $I_{x,y,z}$

↦ commuting set of angular variables I^2, I_3, I_z

total, intrinsic, space-fixed

$I_3 \to K \equiv$ eigenvalue of I_3 $\quad K = -I, \ldots I$

1A-6a Components of angular momentum with respect to intrinsic axes

We label the intrinsic axes by $\kappa = 1, 2, 3$, and the spherical angular momentum components I'_ν with respect to the intrinsic frame are thus

$$I'_{\nu=\pm 1} = \mp \frac{1}{\sqrt{2}}(I_1 \pm iI_2)$$
$$I'_{\nu=0} = I_3 \qquad \text{(1A-88)}$$

The relation between I'_ν and the components referring to the fixed axes can be expressed in the form (see Eqs. (1A-52) and (1A-40))

$$I_\mu = \sum_\nu \mathscr{D}^1_{\mu\nu}(\omega) I'_\nu = \sum_\nu I'_\nu \mathscr{D}^1_{\mu\nu}(\omega)$$
$$I'_\nu = \sum_\mu \mathscr{D}^{1\dagger}_{\mu\nu}(\omega) I_\mu = \sum_\mu I_\mu \mathscr{D}^{1\dagger}_{\mu\nu}(\omega) \qquad \text{(1A-89)}$$

The operators I_μ and I'_ν do not commute with the orientation angles, but the sums in Eq. (1A-89) are independent of the ordering of the $\mathscr{D}$ functions and I components, as can be seen from Eq. (1A-55) with $T_{\lambda\mu} = \mathscr{D}^\lambda_{\mu\nu}$.

Commutation relations involving the I'_ν can be found by applying Eq. (1A-64) to the spherical tensors $\mathscr{D}^\lambda_{\mu\nu}$ and I_μ,

$$[I'_\nu, I_\mu] = 0$$
$$[I'_\nu, \mathscr{D}^\lambda_{\mu\nu'}(\omega)] = (-1)^\nu(\lambda(\lambda+1))^{1/2}\langle \lambda\nu' 1 -\nu | \lambda, \nu'-\nu\rangle \mathscr{D}^\lambda_{\mu,\nu'-\nu}(\omega) \qquad \text{(1A-90)}$$
$$[I'_\nu, I'_{\nu'}] = \sqrt{2}\langle 1\nu 1\nu' | 1, \nu+\nu'\rangle I'_{\nu+\nu'}$$

In terms of the Cartesian components, I_κ, the two last relations in Eq. (1A-90) can be written

$$[I_1, I_2] = -iI_3 \quad \text{and cyclic permutations}$$
$$[I_1 \pm iI_2, \mathscr{D}^\lambda_{\mu\nu}(\omega)] = ((\lambda\pm\nu)(\lambda\mp\nu+1))^{1/2}\mathscr{D}^\lambda_{\mu,\nu\mp1}(\omega) \qquad \text{(1A-91)}$$
$$[I_3, \mathscr{D}^\lambda_{\mu\nu}(\omega)] = \nu \mathscr{D}^\lambda_{\mu\nu}(\omega)$$

→ commutation rules of the intrinsic components

The commutation of I'_ν with I_μ is a simple consequence of the fact that the I'_ν components are independent of the orientation of the external system, and thus scalars with respect to the rotations generated by the I_μ. The commutation relations of the

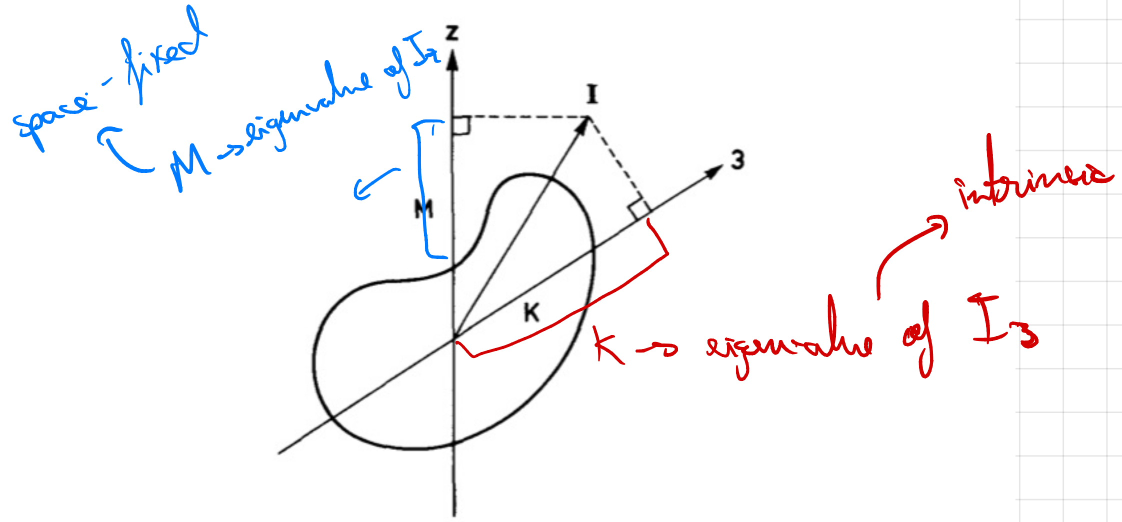


Figure 4-1 Angular momentum quantum numbers describing rotational motion in three dimensions. The z axis belongs to a coordinate system fixed in the laboratory, while the 3 axis is part of a body-fixed coordinate system (compare the $\mathscr{K}$ and $\mathscr{K}'$ systems defined in Fig. 1A-1, Vol. I, p. 76).

$$\varphi_{IKM}(\omega) = \left(\frac{2I+1}{8\pi^2}\right)^{1/2} \mathscr{D}^I_{MK}(\omega) \qquad \text{(4-7)}$$

Wave functions describing orientation of intrinsic system

$\{\phi, \theta, \psi\}$

↓ Euler angles

-system $\xrightarrow{\text{body-fixed}}_{\text{c.s.}}$ state of orientation

$|IKM\rangle \equiv$ conjugates of ω

$\{|\omega\rangle\} \xrightarrow{T} \{|IKM\rangle\}$

sharply defined orientation

$$\mathscr{R}(\omega) = \exp\{-i\phi I_z\}\exp\{-i\theta I_y\}\exp\{-i\psi I_z\} \quad \text{(1A-32)}$$

①

$$\boxed{|IM'\rangle_{R_1} = \sum_M |IM\rangle_{R_0}\, \langle IM|R(\omega)|IM'\rangle}$$

②

$$\mathscr{D}^I_{MM'}(\omega) \equiv \langle IM|\mathscr{R}(\omega)|IM'\rangle^* = \langle IM'|\exp\{i\psi I_z\}\exp\{i\theta I_y\}\exp\{i\phi I_z\}|IM\rangle \quad \text{(1A-33)}$$

$D^I_{MM'}$ ↳ wigner-D functions

normalization

③

The $\mathscr{D}$ functions form a complete orthogonal set of basis functions in ϕ, θ, ψ space, with the normalization

$$\int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\phi \int_0^{2\pi} d\psi\, \mathscr{D}^{I*}_{MM'}(\omega)\mathscr{D}^{I_1}_{M_1M'_1}(\omega) = \frac{8\pi^2}{2I+1}\delta(I,I_1)\,\delta(M,M_1)\,\delta(M',M'_1) \quad \text{(1A-41)}$$

$$\boxed{|\alpha IM\rangle_{\mathscr{K}} = \sum_{M'} \mathscr{D}^I_{MM'}(\omega)\,|\alpha IM'\rangle_{\mathscr{K}'}}$$

$$\varphi_{IKM}(\omega) = \left(\frac{2I+1}{8\pi^2}\right)^{\frac{1}{2}} D^I_{MK}(\omega)$$

space fixed — intrinsic

$$D^I_{MK} = \langle IM|R(\omega)|IK\rangle$$

$$\boxed{K=0} \Rightarrow D^I_{MK} \rightarrow \varphi_{I,K=0,M}(\omega) = \frac{1}{\sqrt{2\pi}}Y_{IM}(\vartheta,\varphi)$$

- wigner functions ⟶ spherical Harmonics

$K=0 \Rightarrow$ rotational wave-function ≡ angular motion of a point particle without spin

$\boxed{I^2 \; , I_z}$ → constants of motion

$\Updownarrow$

$\hat{H}$ = rotationally invariant

$\Downarrow$

$$[\hat{I}_3, \hat{H}] = f(\alpha_{intr})$$

intrinsic properties

- the stationary states involve a superposition of components with different values of K:

$$\varphi_{\gamma IM}(\omega) = C \cdot \sum_K c_{\gamma I}(K) \mathcal{D}^I_{MK}(\omega)$$

$$\boxed{= \sqrt{\frac{2I+1}{8\pi^2}} \sum_K c_{\gamma I}(K) \mathcal{D}^I_{MK}(\omega)}$$

$c_{\gamma K}(K)$ → depend on the relative magnitude of the moments of inertia

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Revision

$$H = H_{intr}(q, p) + H_{Rot,\alpha}(\underbrace{P_\omega, }_{})$$

↳ define orientation

q, p = coordinates and conjugate momenta

P_ω → conjugate angular momenta

α → intrinsic state

Eigenfunctions of H

state of motion

orientation

$\hookrightarrow$ rotation about a fixed axis M, ϕ

$$\varphi_M(\phi) = \frac{1}{\sqrt{2\pi}} e^{iM\phi}$$

$\omega \to$ orientation

$\boxed{I K M} \to$ state of motion $\to$ conjugate variables of ω

$$\varphi_{IKM}(\phi) = \left(\frac{2I+1}{8\pi^2}\right)^{\frac{1}{2}} \underbrace{D^I_{MK}(\omega)}_{\text{Rotation matrices}}$$

transformation

LAB system | ROTATED SYSTEM (coincide with intrinsic)

$|IKM\rangle$ | $|IKM'\rangle_R$

$$\varphi_{I0M}(\phi) = \frac{1}{2\pi} Y_{IM}(\theta, \varphi) \iff K = 0$$

$\Downarrow$ K - finite

$$\Psi_{\gamma IM}(\omega) = \left(\frac{2I+1}{8\pi^2}\right)^{\frac{1}{2}} \sum_K \underbrace{c_{\gamma I}(K)}_{\text{MOI}} \mathcal{D}^I_{MK}(\omega)$$

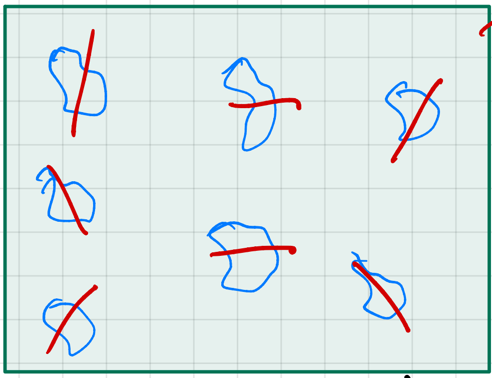
γ = rotational quantum number

4-2b Consequences of Axial Symmetry

If the system possesses axial symmetry, two consequences ensue:

(a) The projection I_3 on the symmetry axis is a constant of the motion.
(b) There are no collective rotations about the symmetry axis.

$K=1,2,3 \Rightarrow$ I_K = c.t. motion $\Leftrightarrow$ K-axis is a symmetry axis



→ • impossible to distinguish orientations of the intrinsic frame that differ only by a rotation about the symmetry axis

intrinsic frame

Axial symmetry $\Leftrightarrow$ NO collective rotations for spherical system

$K \rightarrow$ a.m. of the intrinsic motion

$\boxed{K \rightarrow \text{fixed value}}$

$\alpha \rightarrow$ rotational band