

#### 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  $\phi$ , and the state of motion by the eigenvalue  $M$  of the conjugate angular momentum. The associated rotational wave function is

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

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  $\omega$  (see Sec. 1A-6a). The

→ 2D - rotation

rotation about a fixed axis

6 附

ROTATIONAL SPECTRA Ch. 4

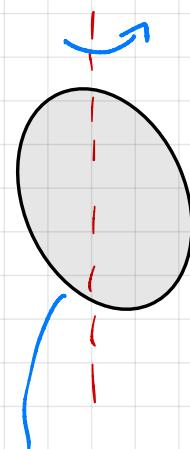
2D-rotation

azimuthal angle  $\phi$

→ orientation

$M \rightarrow$  eigenvalue of the  $\gamma$  angular momentum  
conjugate

↳ state of motion

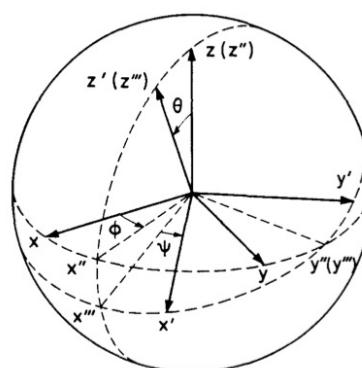


$\omega =$  orientation

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

76 附

ROTATIONAL INVARIANCE App. 1A



3D - rotation

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

# ORIENTATION

$$\omega \rightarrow \phi, \theta, \psi$$

3 angular variables (Euler)

# STATE OF MOTION

3 quantum numbers

①

total angular momentum  $\mathbf{I}$

$I_x = I_x^z$ : component on a space-fixed axis

②

System with orientation  $\omega \rightarrow$  intrinsic C.S.  
 ↳ component of  $\mathbf{I}$  w.r.t. ↗  
 $I_x, K =$  component of  $\mathbf{I}$  on body-fixed c.s.

③

"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

$$J = |j_1 - j_2|, |j_1 - j_2| + 1, \dots, j_1 + j_2 \quad (1A-5)$$

The coupled states  $JM$  can be written in the form

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

$I_{1,2,3} \rightarrow$  - body-fixed

- scalars

- independent of the orientation

$I_{x,y,z} \rightarrow$  - space-fixed

$\rightarrow I_{1,2,3}$  commute with  $I_{x,y,z}$

$\rightarrow$  commuting set of angular variables

total intrinsic space-fixed  
 $\uparrow \quad \uparrow \quad \uparrow$   
 $I^2, I_x, I_y, I_z$

$I_3 \rightarrow K \equiv$  eigenvalue of  $I_3 \quad K = -I, \dots, I$

### IA-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  $I'_\kappa$  with respect to the intrinsic frame are thus

$$I'_{\kappa=\pm 1} = \mp \frac{1}{\sqrt{2}} (I_1 \pm i I_2) \quad (1A-88)$$

$$I'_{\kappa=0} = I_3$$

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

$$I_\mu = \sum_v \mathcal{D}_{\mu v}^1(\omega) I'_v = \sum_v I'_v \mathcal{D}_{\mu v}^1(\omega) \quad (1A-89)$$

$$I'_v = \sum_\mu \mathcal{D}_{\mu v}^{1\dagger}(\omega) I_\mu = \sum_\mu I_\mu \mathcal{D}_{\mu v}^{1\dagger}(\omega)$$

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

Commutation relations involving the  $I'_v$  can be found by applying Eq. (1A-64) to the spherical tensors  $\mathcal{D}_{\mu\nu}^\lambda$  and  $I_\mu$ ,

$$[I'_v, I_\mu] = 0 \quad (1A-90)$$

$$[I'_v, \mathcal{D}_{\mu\nu}^\lambda(\omega)] = (-1)^v (\lambda(\lambda+1))^{1/2} \langle \lambda v' | \lambda, v' - v \rangle \mathcal{D}_{\mu, v'-v}^\lambda(\omega)$$

$$[I'_v, I'_v] = \sqrt{2} \langle 1 v 1 v' | 1, v + v' \rangle I'_{v+v'}$$

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

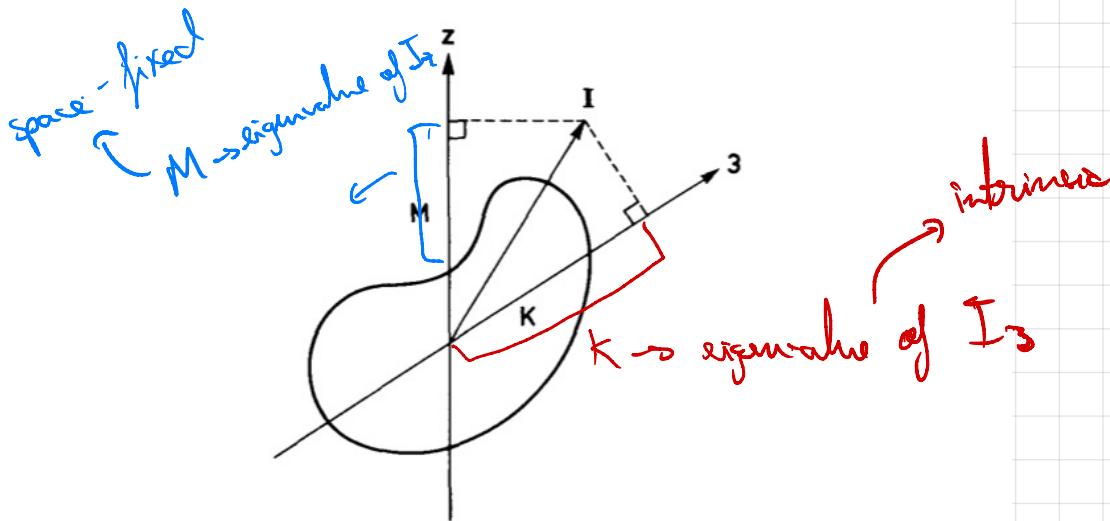
$$[I_1, I_2] = -i I_3 \quad \text{and cyclic permutations} \quad (1A-91)$$

$$[I_1 \pm i I_2, \mathcal{D}_{\mu\nu}^\lambda(\omega)] = ((\lambda \pm v)(\lambda \mp v + 1))^{1/2} \mathcal{D}_{\mu, v\mp 1}^\lambda(\omega)$$

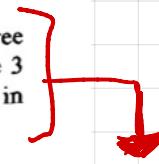
$$[I_3, \mathcal{D}_{\mu\nu}^\lambda(\omega)] = v \mathcal{D}_{\mu\nu}^\lambda(\omega)$$

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

→ commutation rules of  
the intrinsic components



**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  $\mathcal{K}$  and  $\mathcal{K}'$  systems defined in Fig. 1A-1, Vol. I, p. 76).



$$\varphi_{IKM}(\omega) = \left( \frac{2I+1}{8\pi^2} \right)^{1/2} \mathcal{D}_{MK}^I(\omega) \quad (4-7)$$

Wave functions describing orientation of intrinsic system

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

$|IKM\rangle$  = conjugates of  $w$

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

↓ Euler angles

$w$

$$\{ |w\rangle \} \xrightarrow{T} \{ |IM\rangle \}$$

sharply defined orientation

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

$$\textcircled{1} \quad \langle IM' \rangle_{R_1} = \sum_M \langle IM \rangle_{R_0} \in \langle IM | R(\omega) | IM' \rangle$$

\textcircled{2}

$$\mathcal{D}_{MM'}^I(\omega) \equiv \langle IM | \mathcal{R}(\omega) | IM' \rangle^*$$

$$= \langle IM' | \exp\{i\psi I_z\} \exp\{i\theta I_y\} \exp\{i\phi I_z\} | IM \rangle$$

(1A-33)

normalization  
 $D_{MM'}^I$

$\hookrightarrow$  wigner-D functions

\textcircled{3}

The  $D$  functions form a complete orthogonal set of basis functions in  $\phi, \theta, \psi$  space, with the normalization

$$\int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \int_0^{2\pi} d\psi D_{MM'}^I(\omega) D_{M'M'}^{I'}(\omega) \\ = \frac{8\pi^2}{2I+1} \delta(I, I') \delta(M, M') \delta(M', M'')$$

(1A-41)

$$|\alpha IM\rangle_{\mathcal{K}} = \sum_{M'} \mathcal{D}_{MM'}^I(\omega) |\alpha IM'\rangle_{\mathcal{K}'}$$