Chapter 13
Rotational Motion

An asymmetric top under the influence of time dependent external forces is a rather complicated subject in mechanics. Efficient methods to describe the rotational motion are important as well in astrophysics as in molecular physics. The orientation of a rigid body relative to the laboratory system can be described by a 3×3 matrix. Instead of solving nine equations for all its components, the rotation matrix can be parametrized by the four real components of a quaternion. Euler angles use the minimum necessary number of three parameters but have numerical disadvantages. Care has to be taken to conserve the orthogonality of the rotation matrix. Omelyan's implicit quaternion method is very efficient and conserves orthogonality exactly. In computer experiments we compare different explicit and implicit methods for a free rotor, we simulate a rotor in an external field and the collision of two rotating molecules.

13.1 Transformation to a Body Fixed Coordinate System

Let us define a rigid body as a set of mass points m_i with fixed relative orientation (described by distances and angles).

The position of m_i in the laboratory coordinate system CS will be denoted by $\mathbf{r}_i$. The position of the center of mass (COM) of the rigid body is

$$\mathbf{R} = \frac{1}{\sum_i m_i} \sum_i m_i \mathbf{r}_i \tag{13.1}$$

and the position of m_i within the COM coordinate system CS_c (Fig. 13.1) is $\boldsymbol{\rho}_i$:

$$\mathbf{r}_i = \mathbf{R} + \boldsymbol{\rho}_i. \tag{13.2}$$

Let us define a body fixed coordinate system CS_{cb}, where the position $\boldsymbol{\rho}_{ib}$ of m_i is time independent $\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\rho}_{ib} = 0$. $\boldsymbol{\rho}_i$ and $\boldsymbol{\rho}_{ib}$ are connected by a linear vector function

$$\boldsymbol{\rho}_i = A\boldsymbol{\rho}_{ib} \tag{13.3}$$

P.O.J. Scherer, *Computational Physics*, Graduate Texts in Physics,
DOI 10.1007/978-3-319-00401-3_13,

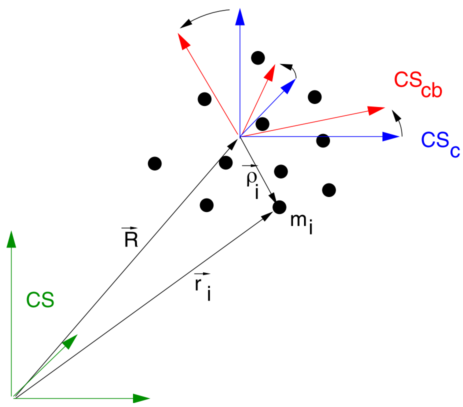


Fig. 13.1 (Coordinate systems) Three coordinate systems will be used: The laboratory system CS, the center of mass system CS_c and the body fixed system CS_{cb}

where A is a 3×3 matrix

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}. \tag{13.4}$$

13.2 Properties of the Rotation Matrix

Rotation conserves the length of $\boldsymbol{\rho}$:[1]

$$\boldsymbol{\rho}^T \boldsymbol{\rho} = (A\boldsymbol{\rho})^T (A\boldsymbol{\rho}) = \boldsymbol{\rho}^T A^T A \boldsymbol{\rho}. \tag{13.5}$$

Consider the matrix

$$M = A^T A - 1 \tag{13.6}$$

for which

$$\boldsymbol{\rho}^T M \boldsymbol{\rho} = 0 \tag{13.7}$$

holds for all vectors $\boldsymbol{\rho}$. Let us choose the unit vector in x-direction:

$$\boldsymbol{\rho} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}.$$

Then we have

$$0 = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = M_{11}. \tag{13.8}$$

[1] $\boldsymbol{\rho}^T \boldsymbol{\rho}$ denotes the scalar product of two vectors whereas $\boldsymbol{\rho}\boldsymbol{\rho}^T$ is the outer or matrix product.

Similarly by choosing a unit vector in y or z direction we find $M_{22} = M_{33} = 0$.

Now choose $\boldsymbol{\rho} = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$:

$$0 = \begin{pmatrix} 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} M_{11} + M_{12} \\ M_{21} + M_{22} \\ M_{31} + M_{32} \end{pmatrix} = M_{11} + M_{22} + M_{12} + M_{21}. \tag{13.9}$$

Since the diagonal elements vanish we have $M_{12} = -M_{21}$. With

$$\boldsymbol{\rho} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \qquad \boldsymbol{\rho} = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

we find $M_{13} = -M_{31}$ and $M_{23} = -M_{32}$, hence M is skew symmetric and has three independent components

$$M = -M^T = \begin{pmatrix} 0 & M_{12} & M_{13} \\ -M_{12} & 0 & M_{23} \\ -M_{13} & -M_{23} & 0 \end{pmatrix}. \tag{13.10}$$

Inserting (13.6) we have

$$\left(A^T A - 1\right) = -\left(A^T A - 1\right)^T = -\left(A^T A - 1\right) \tag{13.11}$$

which shows that $A^T A = 1$ or equivalently $A^T = A^{-1}$. Hence $(\det(A))^2 = 1$ and A is an orthogonal matrix. For a pure rotation without reflection only $\det(A) = +1$ is possible.

From

$$\mathbf{r}_i = \mathbf{R} + A\boldsymbol{\rho}_{ib} \tag{13.12}$$

we calculate the velocity

$$\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t} = \frac{\mathrm{d}\mathbf{R}}{\mathrm{d}t} + \frac{\mathrm{d}A}{\mathrm{d}t}\boldsymbol{\rho}_{ib} + A\frac{\mathrm{d}\boldsymbol{\rho}_{ib}}{\mathrm{d}t} \tag{13.13}$$

but since $\boldsymbol{\rho}_{ib}$ is constant by definition, the last summand vanishes

$$\dot{\mathbf{r}}_i = \dot{\mathbf{R}} + \dot{A}\boldsymbol{\rho}_{ib} = \dot{\mathbf{R}} + \dot{A}A^{-1}\boldsymbol{\rho}_i \tag{13.14}$$

and in the center of mass system we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\rho}_i = \dot{A}A^{-1}\boldsymbol{\rho}_i = W\boldsymbol{\rho}_i \tag{13.15}$$

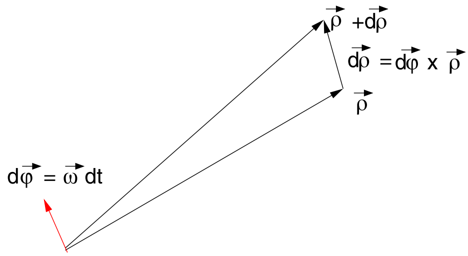


Fig. 13.2 Infinitesimal rotation

with the matrix

$$W = \dot{A}A^{-1}. \tag{13.16}$$

13.3 Properties of W, Connection with the Vector of Angular Velocity

Since rotation does not change the length of $\boldsymbol{\rho}_i$, we have

$$0 = \frac{\mathrm{d}}{\mathrm{d}t}|\boldsymbol{\rho}_i|^2 \to 0 = \boldsymbol{\rho}_i \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\rho}_i = \boldsymbol{\rho}_i(W\boldsymbol{\rho}_i) \tag{13.17}$$

or in matrix notation

$$0 = \boldsymbol{\rho}_i^T W \boldsymbol{\rho}_i. \tag{13.18}$$

This holds for arbitrary $\boldsymbol{\rho}_i$. Hence W is skew symmetric and has three independent components

$$W = \begin{pmatrix} 0 & W_{12} & W_{13} \\ -W_{12} & 0 & W_{23} \\ -W_{13} & -W_{23} & 0 \end{pmatrix}. \tag{13.19}$$

Now consider an infinitesimal rotation by the angle $\mathrm{d}\varphi$ (Fig. 13.2).

Then we have (the index i is suppressed)

$$d\boldsymbol{\rho} = \frac{\mathrm{d}\boldsymbol{\rho}}{\mathrm{d}t}dt = \begin{pmatrix} 0 & W_{12} & W_{13} \\ -W_{12} & 0 & W_{23} \\ -W_{13} & -W_{23} & 0 \end{pmatrix}\begin{pmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \end{pmatrix} dt = \begin{pmatrix} W_{12}\rho_2 + W_{13}\rho_3 \\ -W_{12}\rho_1 + W_{23}\rho_3 \\ -W_{13}\rho_1 - W_{23}\rho_2 \end{pmatrix} dt \tag{13.20}$$

which can be written as a cross product:

$$d\boldsymbol{\rho} = d\boldsymbol{\varphi} \times \boldsymbol{\rho} \tag{13.21}$$

with

$$d\boldsymbol{\varphi} = \begin{pmatrix} -W_{23}dt \\ W_{13}dt \\ -W_{12}dt \end{pmatrix}. \tag{13.22}$$

But this can be expressed in terms of the angular velocity $\boldsymbol{\omega}$ as

$$d\boldsymbol{\varphi} = \boldsymbol{\omega} dt \tag{13.23}$$

and finally we have

$$d\boldsymbol{\varphi} = \boldsymbol{\omega} dt = \begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix} dt \quad W = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix} \tag{13.24}$$

and the more common form of the equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\rho} = W\boldsymbol{\rho} = \boldsymbol{\omega} \times \boldsymbol{\rho}. \tag{13.25}$$

Example (Rotation around the z-axis) For constant angular velocity $\boldsymbol{\omega}$ the equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\rho} = W\boldsymbol{\rho} \tag{13.26}$$

has the formal solution

$$\boldsymbol{\rho} = \mathrm{e}^{Wt}\boldsymbol{\rho}(0) = A(t)\boldsymbol{\rho}(0). \tag{13.27}$$

The angular velocity vector for rotation around the z-axis is

$$\boldsymbol{\omega} = \begin{pmatrix} 0 \\ 0 \\ \omega_3 \end{pmatrix} \tag{13.28}$$

and

$$W = \begin{pmatrix} 0 & -\omega_3 & 0 \\ \omega_3 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{13.29}$$

Higher powers of W can be easily calculated since

$$W^2 = \begin{pmatrix} -\omega_3^2 & 0 & 0 \\ 0 & -\omega_3^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{13.30}$$

$$W^3 = -\omega_3^2 \begin{pmatrix} 0 & -\omega_3 & 0 \\ \omega_3 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{13.31}$$

etc., and the rotation matrix is obtained from the Taylor series

$$A(t) = \mathrm{e}^{Wt} = 1 + Wt + \frac{1}{2}W^2t^2 + \frac{1}{6}W^3t^3 + \cdots$$
$$= 1 + \begin{pmatrix} \omega_3^2 t^2 & 0 & 0 \\ 0 & \omega_3^2 t^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \left(-\frac{1}{2} + \frac{\omega_3^2 t^2}{24} + \cdots \right)$$
$$+ \begin{pmatrix} 0 & -\omega_3 t & 0 \\ \omega_3 t & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \left(1 - \frac{\omega_3^2 t^2}{6} + \cdots \right)$$
$$= \begin{pmatrix} \cos(\omega_3 t) & -\sin(\omega_3 t) & \\ \sin(\omega_3 t) & \cos(\omega_3 t) & \\ & & 1 \end{pmatrix}. \tag{13.32}$$

13.4 Transformation Properties of the Angular Velocity

Now imagine we are sitting on the rigid body and observe a mass point moving outside. Its position in the laboratory system is $\mathbf{r}_1$. In the body fixed system we observe it at

$$\boldsymbol{\rho}_{1b} = A^{-1}(\mathbf{r}_1 - \mathbf{R}) \tag{13.33}$$

and its velocity in the body fixed system is

$$\dot{\boldsymbol{\rho}}_{1b} = A^{-1}(\dot{\mathbf{r}}_1 - \dot{\mathbf{R}}) + \frac{\mathrm{d}A^{-1}}{\mathrm{d}t}(\mathbf{r}_1 - \mathbf{R}). \tag{13.34}$$

The time derivative of the inverse matrix follows from

$$0 = \frac{\mathrm{d}}{\mathrm{d}t}\left(A^{-1}A\right) = A^{-1}\dot{A} + \frac{\mathrm{d}A^{-1}}{\mathrm{d}t}A \tag{13.35}$$

$$\frac{\mathrm{d}A^{-1}}{\mathrm{d}t} = -A^{-1}\dot{A}A^{-1} = -A^{-1}W \tag{13.36}$$

and hence

$$\frac{\mathrm{d}A^{-1}}{\mathrm{d}t}(\mathbf{r}_1 - \mathbf{R}) = -A^{-1}W(\mathbf{r}_1 - \mathbf{R}). \tag{13.37}$$

Now we rewrite this using the angular velocity as it is observed in the body fixed system

$$-A^{-1}W(\mathbf{r}_1 - \mathbf{R}) = -W_b A^{-1}(\mathbf{r}_1 - \mathbf{R}) = -W_b \boldsymbol{\rho}_{1b} = -\boldsymbol{\omega}_b \times \boldsymbol{\rho}_{1b} \tag{13.38}$$

where W transforms as like a rank-2 tensor

$$W_b = A^{-1} W A. \tag{13.39}$$

From this equation the transformation properties of $\boldsymbol{\omega}$ can be derived. We consider only rotation around one axis explicitly, since a general rotation matrix can always be written as a product of three rotations around different axes. For instance, rotation around the z-axis gives:

$$\begin{aligned}
W_b &= \begin{pmatrix} 0 & -\omega_{b3} & \omega_{b2} \\ \omega_{b3} & 0 & -\omega_{b1} \\ -\omega_{b2} & \omega_{b1} & 0 \end{pmatrix} \\
&= \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix} \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \\
&= \begin{pmatrix} 0 & -\omega_3 & \omega_2\cos\varphi - \omega_1\sin\varphi \\ \omega_3 & 0 & -(\omega_1\cos\varphi + \omega_2\sin\varphi) \\ -(\omega_2\cos\varphi - \omega_1\sin\varphi) & \omega_1\cos\varphi + \omega_2\sin\varphi & 0 \end{pmatrix}
\end{aligned} \tag{13.40}$$

which shows that

$$\begin{pmatrix} \omega_{1b} \\ \omega_{2b} \\ \omega_{3b} \end{pmatrix} = \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix} = A^{-1}\boldsymbol{\omega} \tag{13.41}$$

i.e. $\boldsymbol{\omega}$ transforms like a vector under rotations. However, there is a subtle difference considering general coordinate transformations involving reflections. For example, under reflection at the xy-plane W is transformed according to

$$\begin{aligned}
W_b &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \\
&= \begin{pmatrix} 0 & -\omega_3 & -\omega_2 \\ \omega_3 & 0 & \omega_1 \\ \omega_2 & -\omega_1 & 0 \end{pmatrix}
\end{aligned} \tag{13.42}$$

and the transformed angular velocity vector is

$$\begin{pmatrix} \omega_{1b} \\ \omega_{2b} \\ \omega_{3b} \end{pmatrix} = -\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix}. \tag{13.43}$$

This is characteristic of a so called axial or pseudo-vector. Under a general coordinate transformation it transforms as

$$\boldsymbol{\omega}_b = \det(A) A \boldsymbol{\omega}. \tag{13.44}$$

13.5 Momentum and Angular Momentum

The total momentum is

$$\mathbf{P} = \sum_i m_i \dot{\mathbf{r}}_i = \sum_i m_i \dot{\mathbf{R}} = M\dot{\mathbf{R}} \tag{13.45}$$

since by definition we have $\sum_i m_i \boldsymbol{\rho}_i = 0$.

The total angular momentum can be decomposed into the contribution of the center of mass motion and the contribution relative to the center of mass

$$\mathbf{L} = \sum_i m_i \mathbf{r}_i \times \dot{\mathbf{r}}_i = M\mathbf{R} \times \dot{\mathbf{R}} + \sum_i m_i \boldsymbol{\rho}_i \times \dot{\boldsymbol{\rho}}_i = \mathbf{L}_{COM} + \mathbf{L}_{int}. \tag{13.46}$$

The second contribution is

$$\mathbf{L}_{int} = \sum_i m_i \boldsymbol{\rho}_i \times (\boldsymbol{\omega} \times \boldsymbol{\rho}_i) = \sum_i m_i \big(\boldsymbol{\omega}\rho_i^2 - \boldsymbol{\rho}_i(\boldsymbol{\rho}_i\boldsymbol{\omega})\big). \tag{13.47}$$

This is a linear vector function of $\boldsymbol{\omega}$, which can be expressed simpler by introducing the tensor of inertia

$$I = \sum_i m_i \rho_i^2 1 - m_i \boldsymbol{\rho}_i \boldsymbol{\rho}_i^T \tag{13.48}$$

or component-wise

$$I_{m,n} = \sum_i m_i \rho_i^2 \delta_{m,n} - m_i \rho_{i,m} \rho_{i,n} \tag{13.49}$$

as

$$\mathbf{L}_{int} = I\boldsymbol{\omega}. \tag{13.50}$$

13.6 Equations of Motion of a Rigid Body

Let $\mathbf{F}_i$ be an external force acting on m_i. Then the equation of motion for the center of mass is

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} \sum_i m_i \mathbf{r}_i = M\ddot{\mathbf{R}} = \sum_i \mathbf{F}_i = \mathbf{F}_{ext}. \tag{13.51}$$

If there is no total external force $\mathbf{F}_{ext}$, the center of mass moves with constant velocity

$$\mathbf{R} = \mathbf{R}_0 + \mathbf{V}(t - t_0). \tag{13.52}$$

The time derivative of the angular momentum equals the total external torque

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{L} = \frac{\mathrm{d}}{\mathrm{d}t} \sum_i m_i \mathbf{r}_i \times \dot{\mathbf{r}}_i = \sum_i m_i \mathbf{r}_i \times \ddot{\mathbf{r}}_i = \sum_i \mathbf{r}_i \times \mathbf{F}_i = \sum_i \mathbf{N}_i = \mathbf{N}_{ext} \tag{13.53}$$

which can be decomposed into

$$\mathbf{N}_{ext} = \mathbf{R} \times \mathbf{F}_{ext} + \sum_i \boldsymbol{\rho}_i \times \mathbf{F}_i. \tag{13.54}$$

With the decomposition of the angular momentum

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{L} = \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{L}_{COM} + \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{L}_{int} \tag{13.55}$$

we have two separate equations for the two contributions:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{L}_{COM} = \frac{\mathrm{d}}{\mathrm{d}t}M\mathbf{R} \times \dot{\mathbf{R}} = M\mathbf{R} \times \ddot{\mathbf{R}} = \mathbf{R} \times \mathbf{F}_{ext} \tag{13.56}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{L}_{int} = \sum_i \boldsymbol{\rho}_i \times \mathbf{F}_i = \mathbf{N}_{ext} - \mathbf{R} \times \mathbf{F}_{ext} = \mathbf{N}_{int}. \tag{13.57}$$

13.7 Moments of Inertia

The angular momentum (13.50) is

$$\mathbf{L}_{rot} = I\boldsymbol{\omega} = AA^{-1}IAA^{-1}\boldsymbol{\omega} = AI_b\boldsymbol{\omega}_b \tag{13.58}$$

where the tensor of inertia in the body fixed system is

$$\begin{aligned} I_b &= A^{-1}IA = A^{-1}\left(\sum_i m_i \boldsymbol{\rho}_i^T \rho_i - m_i \boldsymbol{\rho}_i \boldsymbol{\rho}_i^T\right)A \\ &= \sum_i m_i A^T \boldsymbol{\rho}_i^T \boldsymbol{\rho}_i A - m_i A^T \boldsymbol{\rho}_i \boldsymbol{\rho}_i^T A \\ &= \sum_i m_i \rho_{ib}^2 - m_i \boldsymbol{\rho}_{ib} \boldsymbol{\rho}_{ib}^T. \end{aligned} \tag{13.59}$$

Since I_b does not depend on time (by definition of the body fixed system) we will use the principal axes of I_b as the axes of the body fixed system. Then I_b takes the simple form

$$I_b = \begin{pmatrix} I_1 & 0 & 0 \\ 0 & I_2 & 0 \\ 0 & 0 & I_3 \end{pmatrix} \tag{13.60}$$

with the principle moments of inertia $I_{1,2,3}$.

13.8 Equations of Motion for a Rotor

The following equations describe pure rotation of a rigid body:

$$\frac{\mathrm{d}}{\mathrm{d}t}A = WA = AW_b \tag{13.61}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{L}_{int} = \mathbf{N}_{int} \tag{13.62}$$

$$W = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix} \qquad W_{ij} = -\varepsilon_{ijk}\omega_k \tag{13.63}$$

$$\mathbf{L}_{int} = A\mathbf{L}_{int,b} = I\omega = AI_b\boldsymbol{\omega}_b \tag{13.64}$$

$$\boldsymbol{\omega}_b = I_b^{-1}\mathbf{L}_{int,b} = \begin{pmatrix} I_1^{-1} & 0 & 0 \\ 0 & I_2^{-1} & 0 \\ 0 & 0 & I_3^{-1} \end{pmatrix}\mathbf{L}_{int,b} \quad \boldsymbol{\omega} = A\boldsymbol{\omega}_b \tag{13.65}$$

$$I_b = \text{const.} \tag{13.66}$$

13.9 Explicit Methods

Equation (13.61) for the rotation matrix and (13.62) for the angular momentum have to be solved by a suitable algorithm. The simplest integrator is the explicit Euler method (Fig. 13.3) [241]:

$$A(t+\Delta t) = A(t) + A(t)W_b(t)\Delta t + O\big(\Delta t^2\big) \tag{13.67}$$

$$\mathbf{L}_{int}(t+\Delta t) = \mathbf{L}_{int}(t) + \mathbf{N}_{int}(t)\Delta t + O\big(\Delta t^2\big). \tag{13.68}$$

Expanding the Taylor series of $A(t)$ to second order we have the second order approximation (Fig. 13.3)

$$A(t+\Delta t) = A(t) + A(t)W_b(t)\Delta t + \frac{1}{2}\big(A(t)W_b^2(t) + A(t)\dot{W}_b(t)\big)\Delta t^2 + O\big(\Delta t^3\big). \tag{13.69}$$

A corresponding second order expression for the angular momentum involves the time derivative of the forces and is usually not practicable.

The time derivative of W can be expressed via the time derivative of the angular velocity which can be calculated as follows:

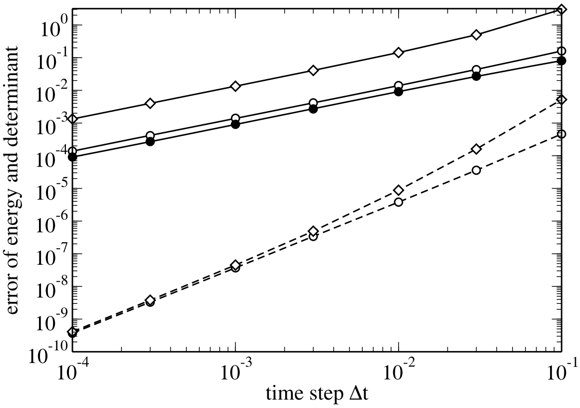


Fig. 13.3 (Global error of the explicit methods) The equations of a free rotor (13.8) are solved using the explicit first order (*full curves*) and second order (*dashed curves*) method. The deviations $|\det(A) - 1|$ (*diamonds*) and $|E_{kin} - E_{kin}(0)|$ (*circles*) at $t = 10$ are shown as a function of the time step Δt. *Full circles* show the energy deviation of the first order method with reorthogonalization. The principal moments of inertia are $I_b = \mathrm{diag}(1, 2, 3)$ and the initial angular momentum is $\mathbf{L} = (1, 1, 1)$. See also Problem 13.1

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\omega}_b &= \frac{\mathrm{d}}{\mathrm{d}t}\big(I_b^{-1}A^{-1}\mathbf{L}_{int}\big) = I_b^{-1}\left(\frac{\mathrm{d}}{\mathrm{d}t}A^{-1}\right)\mathbf{L}_{int} + I_b^{-1}A^{-1}\mathbf{N}_{int} \\ &= I_b^{-1}\big(-A^{-1}W\big)\mathbf{L}_{int} + I_b^{-1}A^{-1}\mathbf{N}_{int} \\ &= -I_b^{-1}W_b\mathbf{L}_{int,b} + I_b^{-1}\mathbf{N}_{int,b}. \end{aligned} \tag{13.70}$$

Alternatively, in the laboratory system

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\omega} &= \frac{\mathrm{d}}{\mathrm{d}t}(A\boldsymbol{\omega}_b) = WA\omega_b - AI_b^{-1}A^{-1}W\mathbf{L}_{int} + AI_b^{-1}A^{-1}\mathbf{N}_{int} \\ &= AI_b^{-1}A(\mathbf{N}_{int} - W\mathbf{L}_{int})\end{aligned} \tag{13.71}$$

where the first summand vanishes due to

$$WA\boldsymbol{\omega}_b = AW_b\boldsymbol{\omega}_b = A\boldsymbol{\omega}_b \times \boldsymbol{\omega}_b = 0. \tag{13.72}$$

Substituting the angular momentum we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\omega}_b = I_b^{-1}\mathbf{N}_{int,b} - I_b^{-1}W_bI_b\boldsymbol{\omega}_b \tag{13.73}$$

which reads in components:

$$\begin{pmatrix} \dot{\omega}_{b1} \\ \dot{\omega}_{b2} \\ \dot{\omega}_{b3} \end{pmatrix} = \begin{pmatrix} I_{b1}^{-1} N_{b1} \\ I_{b2}^{-1} N_{b2} \\ I_{b3}^{-1} N_{b3} \end{pmatrix} - \begin{pmatrix} I_{b1}^{-1} & & \\ & I_{b2}^{-1} & \\ & & I_{b3}^{-1} \end{pmatrix} \begin{pmatrix} 0 & -\omega_{b3} & \omega_{b2} \\ \omega_{b3} & 0 & -\omega_{b1} \\ -\omega_{b2} & \omega_{b1} & 0 \end{pmatrix} \begin{pmatrix} I_{b1}\omega_{b1} \\ I_{b2}\omega_{b2} \\ I_{b3}\omega_{b3} \end{pmatrix}. \tag{13.74}$$

Evaluation of the product gives a set of equations which are well known as Euler's equations:

$$\begin{aligned} \dot{\omega}_{b1} &= \frac{I_{b2} - I_{b3}}{I_{b1}} \omega_{b2}\omega_{b3} + \frac{N_{b1}}{I_{b1}} \\ \dot{\omega}_{b2} &= \frac{I_{b3} - I_{b1}}{I_{b2}} \omega_{b3}\omega_{b1} + \frac{N_{b2}}{I_{b2}} \\ \dot{\omega}_{b3} &= \frac{I_{b1} - I_{b2}}{I_{b3}} \omega_{b1}\omega_{b2} + \frac{N_{b3}}{I_{b3}}. \end{aligned} \tag{13.75}$$

13.10 Loss of Orthogonality

The simple methods above do not conserve the orthogonality of A. This is an effect of higher order but the error can accumulate quickly. Consider the determinant of A. For the simple explicit Euler scheme we have

$$\begin{aligned} \det(A + \Delta A) &= \det(A + WA\Delta t) = \det A \det(1 + W\Delta t) \\ &= \det A\left(1 + \omega^2 \Delta t^2\right). \end{aligned} \tag{13.76}$$

The error is of order Δt^2, but the determinant will continuously increase, i.e. the rigid body will explode. For the second order integrator we find

$$\begin{aligned} \det(A + \Delta A) &= \det\left(A + WA\Delta t + \frac{\Delta t^2}{2}\left(W^2 A + \dot{W} A\right)\right) \\ &= \det A \det\left(1 + W\Delta t + \frac{\Delta t^2}{2}\left(W^2 + \dot{W}\right)\right). \end{aligned} \tag{13.77}$$

This can be simplified to give

$$\det(A + \Delta A) = \det A\left(1 + \dot{\boldsymbol{\omega}}\boldsymbol{\omega}\Delta t^3 + \cdots\right). \tag{13.78}$$

The second order method behaves somewhat better since the product of angular velocity and acceleration can change in time. To assure that A remains a rotation matrix we must introduce constraints or reorthogonalize A at least after some steps (for instance every time when $|\det(A)-1|$ gets larger than a certain threshold). The following method with a symmetric correction matrix is a very useful alternative [127]. The non-singular square matrix A can be decomposed into the product of an orthonormal matrix $\widetilde{A}$ and a positive semi-definite matrix S

$$A = \widetilde{A} S \tag{13.79}$$

with the positive definite square root of the symmetric matrix $A^T A$

$$S = \left(A^T A\right)^{1/2} \tag{13.80}$$

and

$$\widetilde{A} = A S^{-1} = A\left(A^T A\right)^{-1/2} \tag{13.81}$$

which is orthonormal as can be seen from

$$\widetilde{A}^T \widetilde{A} = \left(S^{-1}\right)^T A^T A S^{-1} = S^{-1} S^2 S^{-1} = 1. \tag{13.82}$$

Since the deviation of A from orthogonality is small, we make the approximations

$$S = 1 + s \tag{13.83}$$

$$A^T A = S^2 \approx 1 + 2s \tag{13.84}$$

$$s \approx \frac{A^T A - 1}{2} \tag{13.85}$$

$$S^{-1} \approx 1 - s \approx 1 + \frac{1 - A^T A}{2} + \cdots \tag{13.86}$$

which can be easily evaluated.

13.11 Implicit Method

The quality of the method can be significantly improved by taking the time derivative at midstep (Fig. 13.4) (12.5):

$$A(t + \Delta t) = A(t) + A\left(t + \frac{\Delta t}{2}\right) W\left(t + \frac{\Delta t}{2}\right)\Delta t + \cdots \tag{13.87}$$

$$\mathbf{L}_{int}(t + \Delta t) = \mathbf{L}_{int}(t) + \mathbf{N}_{int}\left(t + \frac{\Delta t}{2}\right)\Delta t + \cdots . \tag{13.88}$$

Taylor series expansion gives

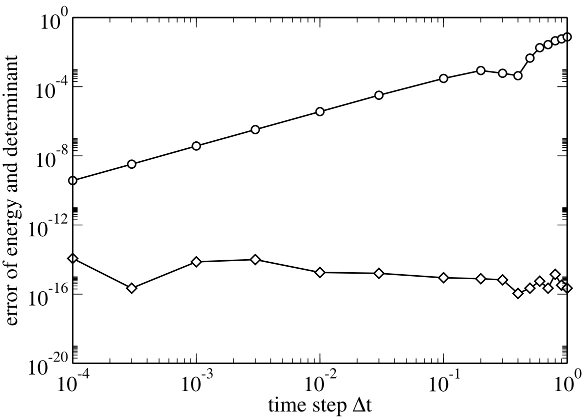


Fig. 13.4 (Global error of the implicit method) The equations of a free rotor (13.8) are solved using the implicit method. The deviations $|\det(A) - 1|$ (*diamonds*) and $|E_{kin} - E_{kin}(0)|$ (*circles*) at $t = 10$ are shown as a function of the time step Δt. Initial conditions as in Fig. 13.3. See also Problem 13.1

$$A\left(t+\frac{\Delta t}{2}\right)W\left(t+\frac{\Delta t}{2}\right)\Delta t$$

$$= A(t)W(t)\Delta t + \dot{A}(t)W(t)\frac{\Delta t^2}{2} + A(t)\dot{W}(t)\frac{\Delta t^2}{2} + O\left(\Delta t^3\right) \quad (13.89)$$

$$= A(t)W(t)\Delta t + \left(A(t)W^2(t) + A(t)\dot{W}(t)\right)\frac{\Delta t^2}{2} + O\left(\Delta t^3\right) \quad (13.90)$$

which has the same error order as the explicit second order method. The matrix $A(t+\frac{\Delta t}{2})$ at mid-time can be approximated by

$$\frac{1}{2}\left(A(t) + A(t+\Delta t)\right) = A\left(t+\frac{\Delta t}{2}\right) + \frac{\Delta t^2}{4}\ddot{A}\left(t+\frac{\Delta t}{2}\right) + \cdots$$

$$= A\left(t+\frac{\Delta t}{2}\right) + O\left(\Delta t^2\right) \quad (13.91)$$

which does not change the error order of the implicit integrator which now becomes

$$A(t+\Delta t) = A(t) + \frac{1}{2}\left(A(t) + A(t+\Delta t)\right)W\left(t+\frac{\Delta t}{2}\right)\Delta t + O\left(\Delta t^3\right). \quad (13.92)$$

This equation can be formally solved by

$$A(t+\Delta t) = A(t)\left(1 + \frac{\Delta t}{2}W\left(t+\frac{\Delta t}{2}\right)\right)\left(1 - \frac{\Delta t}{2}W\left(t+\frac{\Delta t}{2}\right)\right)^{-1}$$

$$= A(t)T_b\left(\frac{\Delta t}{2}\right). \quad (13.93)$$

Alternatively, using angular velocities in the laboratory system we have the similar expression

$$A(t+\Delta t) = \left[1 - \frac{\Delta t}{2} W\left(t + \frac{\Delta t}{2}\right)\right]^{-1} \left[1 + \frac{\Delta t}{2} W\left(t + \frac{\Delta t}{2}\right)\right] A(t)$$
$$= T\left(\frac{\Delta t}{2}\right) A(t). \tag{13.94}$$

The angular velocities at midtime can be calculated with sufficient accuracy from

$$W\left(t + \frac{\Delta t}{2}\right) = W(t) + \frac{\Delta t}{2} \dot{W}(t) + O\left(\Delta t^2\right). \tag{13.95}$$

With the help of an algebra program we easily prove that

$$\det\left(1 + \frac{\Delta t}{2} W\right) = \det\left(1 - \frac{\Delta t}{2} W\right) = 1 + \frac{\omega^2 \Delta t^2}{4} \tag{13.96}$$

and therefore the determinant of the rotation matrix is conserved. The necessary matrix inversion can be easily done:

$$\left[1 - \frac{\Delta t}{2} W\right]^{-1}$$
$$= \begin{pmatrix} 1 + \frac{\omega_1^2 \Delta t^2}{4} & -\omega_3 \frac{\Delta t}{2} + \omega_1 \omega_2 \frac{\Delta t^2}{4} & \omega_2 \frac{\Delta t}{2} + \omega_1 \omega_3 \frac{\Delta t^2}{4} \\ \omega_3 \frac{\Delta t}{2} + \omega_1 \omega_2 \frac{\Delta t^2}{4} & 1 + \frac{\omega_2^2 \Delta t^2}{4} & -\omega_1 \frac{\Delta t}{2} + \omega_2 \omega_3 \frac{\Delta t^2}{4} \\ -\omega_2 \frac{\Delta t}{2} + \omega_1 \omega_3 \frac{\Delta t^2}{4} & \omega_1 \frac{\Delta t}{2} + \omega_2 \omega_3 \frac{\Delta t^2}{4} & 1 + \frac{\omega_3^2 \Delta t^2}{4} \end{pmatrix}$$
$$\times \frac{1}{1 + \omega^2 \frac{\Delta t^2}{4}}. \tag{13.97}$$

The matrix product is explicitly

$$T_b = \left[1 + \frac{\Delta t}{2} W_b\right] \left[1 - \frac{\Delta t}{2} W_b\right]^{-1}$$
$$= \begin{pmatrix} 1 + \frac{\omega_{b1}^2 - \omega_{b2}^2 - \omega_{b3}^2}{4} \Delta t^2 & -\omega_{b3} \Delta t + \omega_{b1} \omega_{b2} \frac{\Delta t^2}{2} & \omega_{b2} \Delta t + \omega_{b1} \omega_{b3} \frac{\Delta t^2}{2} \\ \omega_{b3} \Delta t + \omega_{b1} \omega_{b2} \frac{\Delta t^2}{2} & 1 + \frac{-\omega_{b1}^2 + \omega_{b2}^2 - \omega_{b3}^2}{4} \Delta t^2 & -\omega_{b1} \Delta t + \omega_{b2} \omega_{b3} \frac{\Delta t^2}{2} \\ -\omega_{b2} \Delta t + \omega_{b1} \omega_{b3} \frac{\Delta t^2}{2} & \omega_{b1} \Delta t + \omega_{b2} \omega_{b3} \frac{\Delta t^2}{2} & 1 + \frac{-\omega_{b1}^2 - \omega_{b2}^2 + \omega_{b3}^2}{4} \Delta t^2 \end{pmatrix}$$
$$\times \frac{1}{1 + \omega_b^2 \frac{\Delta t^2}{4}}. \tag{13.98}$$

With the help of an algebra program it can be proved that this matrix is even orthogonal

$$T_b^T T_b = 1 \tag{13.99}$$

and hence the orthonormality of A is conserved. The approximation for the angular momentum

$$\mathbf{L}_{int}(t) + \mathbf{N}_{int}\left(t + \frac{\Delta t}{2}\right)\Delta t$$
$$= \mathbf{L}_{int}(t) + \mathbf{N}_{int}(t)\Delta t + \dot{\mathbf{N}}_{int}(t)\frac{\Delta t^2}{2} + \cdots = \mathbf{L}_{int}(t + \Delta t) + O\left(\Delta t^3\right) \tag{13.100}$$

can be used in an implicit way

$$\mathbf{L}_{int}(t + \Delta t) = \mathbf{L}_{int}(t) + \frac{\mathbf{N}_{int}(t + \Delta t) + \mathbf{N}_{int}(t)}{2}\Delta t + O\left(\Delta t^3\right). \tag{13.101}$$

Alternatively Euler's equations can be used in the form [190, 191]

$$\omega_{b1}\left(t + \frac{\Delta t}{2}\right) = \omega_{b1}\left(t - \frac{\Delta t}{2}\right) + \frac{I_{b2} - I_{b3}}{I_{b1}}\omega_{b2}(t)\omega_{b3}(t)\Delta t + \frac{N_{b1}}{I_{b1}}\Delta t \text{ etc.} \tag{13.102}$$

where the product $\omega_{b2}(t)\omega_{b3}(t)$ is approximated by

$$\omega_{b2}(t)\omega_{b3}(t) = \frac{1}{2}\left[\omega_{b2}\left(t - \frac{\Delta t}{2}\right)\omega_{b3}\left(t - \frac{\Delta t}{2}\right) + \omega_{b2}\left(t + \frac{\Delta t}{2}\right)\omega_{b3}\left(t + \frac{\Delta t}{2}\right)\right]. \tag{13.103}$$

$\omega_{b1}(t + \frac{\Delta t}{2})$ is determined by iterative solution of the last two equations. Starting with $\omega_{b1}(t - \frac{\Delta t}{2})$ convergence is achieved after few iterations.

Example (Free symmetric rotor) For the special case of a free symmetric rotor ($I_{b2} = I_{b3}, \mathbf{N}_{int} = 0$) Euler's equations simplify to:

$$\dot{\omega}_{b1} = 0 \tag{13.104}$$

$$\dot{\omega}_{b2} = \frac{I_{b2(3)} - I_{b1}}{I_{b2(3)}}\omega_{b1}\omega_{b3} = \lambda\omega_{b3} \tag{13.105}$$

$$\dot{\omega}_{b3} = \frac{I_{b1} - I_{b2(3)}}{I_{b2(3)}}\omega_{b1}\omega_{b2} = -\lambda\omega_{b2} \tag{13.106}$$

$$\lambda = \frac{I_{b2(3)} - I_{b1}}{I_{b2(3)}}\omega_{b1}. \tag{13.107}$$

Coupled equations of this type appear often in physics. The solution can be found using a complex quantity

$$\Omega = \omega_{b2} + i\omega_{b3} \tag{13.108}$$

which obeys the simple differential equation

$$\dot{\Omega} = \dot{\omega}_{b2} + i\dot{\omega}_{b3} = -i(i\lambda\omega_{b3} + \lambda\omega_{b2}) = -i\lambda\Omega \tag{13.109}$$

with the solution

$$\Omega = \Omega_0 \mathrm{e}^{-i\lambda t}. \tag{13.110}$$

Finally

$$\boldsymbol{\omega}_b = \begin{pmatrix} \omega_{b1}(0) \\ \Re(\Omega_0 \mathrm{e}^{-i\lambda t}) \\ \Im(\Omega_0 \mathrm{e}^{-i\lambda t}) \end{pmatrix} = \begin{pmatrix} \omega_{b1}(0) \\ \omega_{b2}(0)\cos(\lambda t) + \omega_{b3}(0)\sin(\lambda t) \\ \omega_{b3}(0)\cos(\lambda t) - \omega_{b2}(0)\sin(\lambda t) \end{pmatrix} \tag{13.111}$$

i.e. $\boldsymbol{\omega}_b$ rotates around the 1-axis with frequency λ.

13.12 Kinetic Energy of a Rotor

The kinetic energy of the rotor is

$$\begin{aligned} E_{kin} &= \sum_i \frac{m_i}{2}\dot{r}_i^2 = \sum_i \frac{m_i}{2}(\dot{\mathbf{R}} + \dot{A}\boldsymbol{\rho}_{ib})^2 \\ &= \sum_i \frac{m_i}{2}\left(\dot{R}^T + \boldsymbol{\rho}_{ib}^T \dot{A}^T\right)(\dot{R} + \dot{A}\boldsymbol{\rho}_{ib}) \\ &= \frac{M}{2}\dot{R}^2 + \sum_i \frac{m_i}{2}\boldsymbol{\rho}_{ib}^T \dot{A}^T \dot{A}\boldsymbol{\rho}_{ib}. \end{aligned} \tag{13.112}$$

The second part is the contribution of the rotational motion. It can be written as

$$E_{rot} = \sum_i \frac{m_i}{2}\boldsymbol{\rho}_{ib}^T W_b^T A^T A W_b \boldsymbol{\rho}_{ib} = -\sum_i \frac{m_i}{2}\boldsymbol{\rho}_{ib}^T W_b^2 \boldsymbol{\rho}_{ib} = \frac{1}{2}\omega_b^T I_b \boldsymbol{\omega}_b \tag{13.113}$$

since

$$-W_b^2 = \begin{pmatrix} \omega_{b3}^2 + \omega_{b2}^2 & -\omega_{b1}\omega_{b2} & -\omega_{b1}\omega_{b3} \\ -\omega_{b1}\omega_{b2} & \omega_{b1}^2 + \omega_{b3}^2 & -\omega_{b2}\omega_{b3} \\ -\omega_{b1}\omega_{b3} & -\omega_{b2}\omega_{b3} & \omega_{b1}^2 + \omega_{b2}^2 \end{pmatrix} = \omega_b^2 - \boldsymbol{\omega}_b \boldsymbol{\omega}_b^T. \tag{13.114}$$

13.13 Parametrization by Euler Angles

So far we had to solve equations for all 9 components of the rotation matrix. But there are six constraints since the column vectors of the matrix have to be orthonormalized. Therefore the matrix can be parametrized with less than 9 variables. In fact it is sufficient to use only three variables. This can be achieved by splitting the full rotation into three rotations around different axis. Most common are Euler angles defined by the orthogonal matrix [106]

$$\begin{pmatrix} \cos\psi\cos\phi - \cos\theta\sin\phi\sin\psi & -\sin\psi\cos\phi - \cos\theta\sin\phi\cos\psi & \sin\theta\sin\phi \\ \cos\psi\sin\phi + \cos\theta\cos\phi\sin\psi & -\sin\psi\sin\phi + \cos\theta\cos\phi\cos\psi & -\sin\theta\cos\phi \\ \sin\theta\sin\psi & \sin\theta\cos\psi & \cos\theta \end{pmatrix} \tag{13.115}$$

obeying the equations

$$\dot{\phi} = \omega_x \frac{\sin\phi\cos\theta}{\sin\theta} + \omega_y \frac{\cos\phi\cos\theta}{\sin\theta} + \omega_z \tag{13.116}$$

$$\dot{\theta} = \omega_x \cos\phi + \omega_y \sin\phi \tag{13.117}$$

$$\dot{\psi} = \omega_x \frac{\sin\phi}{\sin\theta} - \omega_y \frac{\cos\phi}{\sin\theta}. \tag{13.118}$$

Different versions of Euler angles can be found in the literature, together with the closely related cardanic angles. For all of them a $\sin\theta$ appears in the denominator which causes numerical instabilities at the poles. One possible solution to this problem is to switch between two different coordinate systems.

13.14 Cayley-Klein Parameters, Quaternions, Euler Parameters

There exists another parametrization of the rotation matrix which is very suitable for numerical calculations. It is connected with the algebra of the so called quaternions. The vector space of the complex 2×2 matrices can be spanned using Pauli matrices by

$$1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{13.119}$$

Any complex 2×2 matrix can be written as a linear combination

$$c_0 1 + \mathbf{c}\boldsymbol{\sigma}. \tag{13.120}$$

Accordingly any vector $\mathbf{x} \in R^3$ can be mapped onto a complex 2×2 matrix:

$$\mathbf{x} \to P = \begin{pmatrix} z & x - iy \\ x + iy & -z \end{pmatrix}. \tag{13.121}$$

Rotation of the coordinate system leads to the transformation

$$P' = QPQ^\dagger \tag{13.122}$$

where

$$Q = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \tag{13.123}$$

is a complex 2×2 rotation matrix. Invariance of the length ($|\mathbf{x}| = \sqrt{-\det(P)}$) under rotation implies that Q must be unitary, i.e. $Q^\dagger = Q^{-1}$ and its determinant must be 1. Explicitly

$$Q^\dagger = \begin{pmatrix} \alpha^* & \gamma^* \\ \beta^* & \delta^* \end{pmatrix} = Q^{-1} = \frac{1}{\alpha\delta - \beta\gamma} \begin{pmatrix} \delta & -\beta \\ -\gamma & \alpha \end{pmatrix} \tag{13.124}$$

and Q has the form

$$Q = \begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix} \quad \text{with } |\alpha|^2 + |\beta|^2 = 1. \tag{13.125}$$

Setting $x_\pm = x \pm iy$, the transformed matrix has the same form as P:

$$\begin{aligned} QPQ^\dagger &= \begin{pmatrix} \alpha^*\beta x_+ + \beta^*\alpha x_- + (|\alpha|^2 - |\beta|^2)z & -\beta^2 x_+ + \alpha^2 x_- - 2\alpha\beta z \\ \alpha^{*2} x_+ - \beta^{*2} x_- - 2\alpha^*\beta^* z & -\alpha^*\beta x_+ - \alpha\beta^* x_- - (|\alpha|^2 - |\beta|^2)z \end{pmatrix} \\ &= \begin{pmatrix} z' & x'_- \\ x'_+ & -z' \end{pmatrix}. \end{aligned} \tag{13.126}$$

From comparison we find the transformed vector components:

$$\begin{aligned} x' &= \frac{1}{2}\left(x'_+ + x'_-\right) = \frac{1}{2}\left(\alpha^{*2} - \beta^2\right)x_+ + \frac{1}{2}\left(\alpha^2 - \beta^{*2}\right)x_- - \left(\alpha\beta + \alpha^*\beta^*\right)z \\ &= \frac{\alpha^{*2} + \alpha^2 - \beta^{*2} - \beta^2}{2}x + \frac{i(\alpha^{*2} - \alpha^2 + \beta^{*2} - \beta^2)}{2}y \\ &\quad - \left(\alpha\beta + \alpha^*\beta^*\right)z \end{aligned} \tag{13.127}$$

$$\begin{aligned} y' &= \frac{1}{2i}\left(x'_+ - x'_-\right) = \frac{1}{2i}\left(\alpha^{*2} + \beta^2\right)x_+ + \frac{1}{2i}\left(-\beta^{*2} - \alpha^2\right)x_- + \frac{1}{i}\left(-\alpha^*\beta^* + \alpha\beta\right)z \\ &= \frac{\alpha^{*2} - \alpha^2 - \beta^{*2} + \beta^2}{2i}x + \frac{\alpha^{*2} + \alpha^2 + \beta^{*2} + \beta^2}{2}y \\ &\quad + i\left(\alpha^*\beta^* - \alpha\beta\right)z \end{aligned} \tag{13.128}$$

$$z' = \left(\alpha^*\beta + \alpha\beta^*\right)x + i\left(\alpha^*\beta - \alpha\beta^*\right)y + \left(|\alpha|^2 - |\beta|^2\right)z. \tag{13.129}$$

This gives us the rotation matrix in terms of the Cayley-Klein parameters α and β:

$$A = \begin{pmatrix} \frac{\alpha^{*2}+\alpha^2-\beta^{*2}-\beta^2}{2} & \frac{i(\alpha^{*2}-\alpha^2+\beta^{*2}-\beta^2)}{2} & -(\alpha\beta + \alpha^*\beta^*) \\ \frac{\alpha^{*2}-\alpha^2-\beta^{*2}+\beta^2}{2i} & \frac{\alpha^{*2}+\alpha^2+\beta^{*2}+\beta^2}{2} & \frac{1}{i}(-\alpha^*\beta^* + \alpha\beta) \\ (\alpha^*\beta + \alpha\beta^*) & i(\alpha^*\beta - \alpha\beta^*) & (|\alpha|^2 - |\beta|^2) \end{pmatrix}. \tag{13.130}$$

For practical calculations one often prefers to have four real parameters instead of two complex ones. The so called Euler parameters q_0, q_1, q_2, q_3 are defined by

$$\alpha = q_0 + iq_3 \qquad \beta = q_2 + iq_1. \tag{13.131}$$

Now the matrix Q

$$Q = \begin{pmatrix} q_0 + iq_3 & q_2 + iq_1 \\ -q_2 + iq_1 & q_0 - iq_3 \end{pmatrix} = q_0 1 + iq_1\sigma_x + iq_2\sigma_y + iq_3\sigma_z \tag{13.132}$$

becomes a so called quaternion which is a linear combination of the four matrices

$$U = 1 \qquad I = i\sigma_z \qquad J = i\sigma_y \qquad K = i\sigma_x \tag{13.133}$$

which obey the following multiplication rules:

$$\begin{aligned} I^2 &= J^2 = K^2 = -U \\ IJ &= -JI = K \\ JK &= -KJ = I \\ KI &= -IK = J. \end{aligned} \tag{13.134}$$

In terms of Euler parameters the rotation matrix reads

$$A = \begin{pmatrix} q_0^2 + q_1^2 - q_2^2 - q_3^2 & 2(q_1q_2 + q_0q_3) & 2(q_1q_3 - q_0q_2) \\ 2(q_1q_2 - q_0q_3) & q_0^2 - q_1^2 + q_2^2 - q_3^2 & 2(q_2q_3 + q_0q_1) \\ 2(q_1q_3 + q_0q_2) & 2(q_2q_3 - q_0q_1) & q_0^2 - q_1^2 - q_2^2 + q_3^2 \end{pmatrix} \tag{13.135}$$

and from the equation $\dot{A} = WA$ we derive the equation of motion for the quaternion

$$\begin{pmatrix} \dot{q}_0 \\ \dot{q}_1 \\ \dot{q}_2 \\ \dot{q}_3 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 & \omega_1 & \omega_2 & \omega_3 \\ -\omega_1 & 0 & -\omega_3 & \omega_2 \\ -\omega_2 & \omega_3 & 0 & -\omega_1 \\ -\omega_3 & -\omega_2 & \omega_1 & 0 \end{pmatrix} \begin{pmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{pmatrix} \tag{13.136}$$

or from $\dot{A} = AW_b$ the alternative equation

$$\begin{pmatrix} \dot{q}_0 \\ \dot{q}_1 \\ \dot{q}_2 \\ \dot{q}_3 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 & \omega_{1b} & \omega_{2b} & \omega_{3b} \\ -\omega_{1b} & 0 & \omega_{3b} & -\omega_{2b} \\ -\omega_{2b} & -\omega_{3b} & 0 & \omega_{1b} \\ -\omega_{3b} & \omega_{2b} & -\omega_{1b} & 0 \end{pmatrix} \begin{pmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{pmatrix}. \tag{13.137}$$

Both of these equations can be written briefly in the form

$$\dot{\mathbf{q}} = \widetilde{W}\mathbf{q}. \tag{13.138}$$

Example (Rotation around the z-axis) Rotation around the z-axis corresponds to the quaternion with Euler parameters

$$\mathbf{q} = \begin{pmatrix} \cos\frac{\omega t}{2} \\ 0 \\ 0 \\ -\sin\frac{\omega t}{2} \end{pmatrix} \tag{13.139}$$

as can be seen from the rotation matrix

$$A = \begin{pmatrix} (\cos\frac{\omega t}{2})^2 - (\sin\frac{\omega t}{2})^2 & -2\cos\frac{\omega t}{2}\sin\frac{\omega t}{2} & 0 \\ 2\cos\frac{\omega t}{2}\sin\frac{\omega t}{2} & (\cos\frac{\omega t}{2})^2 - (\sin\frac{\omega t}{2})^2 & 0 \\ 0 & 0 & (\cos\frac{\omega t}{2})^2 + (\sin\frac{\omega t}{2})^2 \end{pmatrix}$$

$$= \begin{pmatrix} \cos\omega t & -\sin\omega t & 0 \\ \sin\omega t & \cos\omega t & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{13.140}$$

The time derivative of $\mathbf{q}$ obeys the equation

$$\dot{\mathbf{q}} = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & \omega \\ 0 & 0 & -\omega & 0 \\ 0 & \omega & 0 & 0 \\ -\omega & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \cos\frac{\omega t}{2} \\ 0 \\ 0 \\ -\sin\frac{\omega t}{2} \end{pmatrix} = \begin{pmatrix} -\frac{\omega}{2}\sin\omega t \\ 0 \\ 0 \\ -\frac{\omega}{2}\cos\omega t \end{pmatrix}. \tag{13.141}$$

After a rotation by 2π the quaternion changes its sign, i.e. $\mathbf{q}$ and $-\mathbf{q}$ parametrize the same rotation matrix!

13.15 Solving the Equations of Motion with Quaternions

As with the matrix method we can obtain a simple first or second order algorithm from the Taylor series expansion

$$\mathbf{q}(t+\Delta t) = \mathbf{q}(t) + \widetilde{W}(t)\mathbf{q}(t)\Delta t + \big(\dot{\widetilde{W}}(t) + \widetilde{W}^2(t)\big)\mathbf{q}(t)\frac{\Delta t^2}{2} + \cdots. \tag{13.142}$$

Now only one constraint remains, which is the conservation of the norm of the quaternion. This can be taken into account by rescaling the quaternion whenever its norm deviates too much from unity.

It is also possible to use Omelyan's [192] method:

$$\mathbf{q}(t+\Delta t) = \mathbf{q}(t) + \widetilde{W}\left(t + \frac{\Delta t}{2}\right)\frac{1}{2}\big(\mathbf{q}(t) + \mathbf{q}(t+\Delta t)\big) \tag{13.143}$$

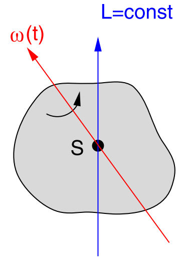
gives

$$\mathbf{q}(t+\Delta t) = \left(1 - \frac{\Delta t}{2}\widetilde{W}\right)^{-1}\left(1 + \frac{\Delta t}{2}\widetilde{W}\right)\mathbf{q}(t) \tag{13.144}$$

where the inverse matrix is

$$\left(1 - \frac{\Delta t}{2}\widetilde{W}\right)^{-1} = \frac{1}{1 + \omega^2\frac{\Delta t^2}{16}}\left(1 + \frac{\Delta t}{2}\widetilde{W}\right) \tag{13.145}$$

Fig. 13.5 Free asymmetric rotor



and the matrix product

$$\left(1-\frac{\Delta t}{2}\widetilde{W}\right)^{-1}\left(1+\frac{\Delta t}{2}\widetilde{W}\right)=\frac{1-\omega^2\frac{\Delta t^2}{16}}{1+\omega^2\frac{\Delta t^2}{16}}+\frac{\Delta t}{1+\omega^2\frac{\Delta t^2}{16}}\widetilde{W}. \tag{13.146}$$

This method conserves the norm of the quaternion and works quite well.

13.16 Problems

Problem 13.1 (Free rotor, Fig. 13.5) In this computer experiment we compare different methods for a free rotor (Sect. 13.8):

- explicit first order method (13.67)

$$A(t+\Delta t)=A(t)+A(t)W_b(t)\Delta t+O\left(\Delta t^2\right) \tag{13.147}$$

- explicit second order method (13.69)

$$A(t+\Delta t)=A(t)+A(t)W_b(t)\Delta t+\frac{1}{2}\left(A(t)W_b^2(t)+A(t)\dot{W}_b(t)\right)\Delta t^2+O\left(\Delta t^3\right) \tag{13.148}$$

- implicit second order method (13.93)

$$A(t+\Delta t)=A(t)\left(1+\frac{\Delta t}{2}W\left(t+\frac{\Delta t}{2}\right)\right)\left(1-\frac{\Delta t}{2}W\left(t+\frac{\Delta t}{2}\right)\right)^{-1}+O\left(\Delta t^3\right). \tag{13.149}$$

The explicit methods can be combined with reorthogonalization according to (13.79) or with the Gram-Schmidt method. Reorthogonalization threshold and time step can be varied and the error of kinetic energy and determinant are plotted as a function of the total simulation time.

Problem 13.2 (Rotor in a field, Fig. 13.6) In this computer experiment we simulate a molecule with a permanent dipole moment in a homogeneous electric field **E**. We neglect vibrations and describe the molecule as a rigid body consisting of nuclei

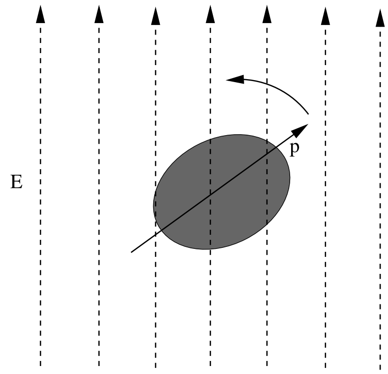


Fig. 13.6 Rotor in an electric field

with masses m_i and partial charges Q_i. The total charge is $\sum_i Q_i = 0$. The dipole moment is

$$\mathbf{p} = \sum_i Q_i \mathbf{r}_i \tag{13.150}$$

and external force and torque are

$$\mathbf{F}_{ext} = \sum_i Q_i \mathbf{E} = 0 \tag{13.151}$$

$$\mathbf{N}_{ext} = \sum_i Q_i \mathbf{r}_i \times \mathbf{E} = \mathbf{p} \times \mathbf{E}. \tag{13.152}$$

The angular momentum changes according to

$$\frac{d}{\Delta t}\mathbf{L}_{int} = \mathbf{p} \times \mathbf{E} \tag{13.153}$$

where the dipole moment is constant in the body fixed system. We use the implicit integrator for the rotation matrix (13.93) and the equation

$$\dot{\boldsymbol{\omega}}_b(t) = -I_b^{-1} W_b(t) \mathbf{L}_{int,b}(t) + I_b^{-1} A^{-1}(t)\big(\mathbf{p}(t) \times \mathbf{E}\big) \tag{13.154}$$

to solve the equations of motion numerically. Obviously the component of the angular momentum parallel to the field is constant. The potential energy is

$$U = -\sum_i Q_i \mathbf{E} \mathbf{r}_i = -\mathbf{p}\mathbf{E}. \tag{13.155}$$

Problem 13.3 (Molecular collision) This computer experiment simulates the collision of two rigid methane molecules (Fig. 13.7). The equations of motion are solved with the implicit quaternion method (13.143) and the velocity Verlet method (12.11.4). The two molecules interact by a standard 6–12 Lennard-Jones potential (14.24) [3]. For comparison the attractive r^{-6} part can be switched off. The initial

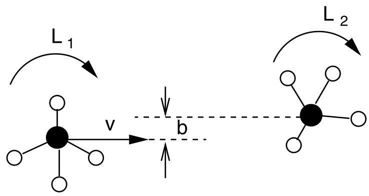


Fig. 13.7 Molecular collision

angular momenta as well as the initial velocity v and collision parameter b can be varied. Total energy and momentum are monitored and the decomposition of the total energy into translational, rotational and potential energy are plotted as a function of time.

Study the exchange of momentum and angular momentum and the transfer of energy between translational and rotational degrees of freedom.