Lecture notes for PC2132 (Classical Mechanics)

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Disclaimer

These notes are by no means a suitable replacement for a proper textbook on classical mechanics, nor should it replace your own notes. It is just a best-effort affair with the intention to be useful.

This is a document in process – it hopefully does not contain too many mistakes, but please contact us if you feel that you spotted one.

Notation

There is an attempt to do use consistent notations through this lecture. Below is a list what symbols typically refer to, unless they are referenced to otherwise.

a	a vector; often the acceleration
e	a unit vector, i.e., a vector of length 1 ($\mathbf{e} \cdot \mathbf{e} = 1$)
$d\mathbf{A}$	a vector differential representing an oriented surface area element
$d\mathbf{s}$	a vector differential representing a line element
${f F}$	a vector representing a force
H	a scalar representing the Hamilton function of a system
$\underline{\underline{\underline{I}}}$	the tensor for the inertia of a rigid body
\overline{L}	a scalar representing the Lagrange function
${f L}$	a vector representing an angular momentum
\mathbf{N}	a vector representing a torque
m	a scalar representing the mass of a particle
$\underline{\underline{\mathbf{m}}}$	mass matrix in a system of coupled masses
M	the total mass of a system
p	a vector representing the momentum $m\mathbf{v}$ of a particle
P	a vector representing the total momentum of a system
q_k	a generalized coordinate
Q	the "quality factor" of a damped harmonic oscillator
\mathbf{r} (or \mathbf{x})	The position of a particle, represented by a vector
S	path length of a trajectory
σ	scattering cross section, has unit of an area
t	time; typically a parameter that parameterizes the evolution of a system
T	either a time like a period or a total time, or a kinetic energy
U	potential energy
V	another vector, often the velocity of a particle
v	a scalar, often referring to the speed $ \mathbf{v} $
W_{12}	a scalar representing work for a state change $1 \rightarrow 2$
$\delta oldsymbol{ heta}$	a vector representing an infinitesimal rotation by an angle $\delta\theta$
Ω	solid angle, characterizes a set of directions, unit sr (steradian)
ω	a vector representing an angular velocity
x_i	the <i>i</i> -th component of a vector \mathbf{x}

1 Kinematics

1.1 Trajectories, velocity, acceleration

This part deals with a geometric description of the trajectories of a single point-like object without going through how such a trajectory comes about.

In its simplest form, the motion of a particle over time can be described as a time-dependent position vector

$$\mathbf{r}(t) = \begin{pmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \end{pmatrix} = \begin{pmatrix} x(t) \\ y(t) \\ z(t) \end{pmatrix}$$
 (1)

This is a representation of the position \mathbf{r} in traditional Cartesian coordinates x, y, z or – to simplify notations later – x_1, x_2, x_3 . In order to prepare ourselves for other coordinate systems, we write this as

$$\mathbf{r}(t) = x_1(t)\,\mathbf{e}_1 + x_2(t)\,\mathbf{e}_2 + x_3(t)\,\mathbf{e}_3 = \sum_{i=1}^3 x_i\mathbf{e}_i\,,\tag{2}$$

where the \mathbf{e}_i are the unit vectors of the standard Cartesian coordinate system. These unit vectors are normalized, which can be expressed by the scalar product, $\mathbf{e}_i \cdot \mathbf{e}_i = 1$, and two \mathbf{e}_i with different indices are orthogonal, i.e., $\mathbf{e}_i \cdot \mathbf{e}_j = 0$ for $i \neq j$. This can be summarized by the short notation

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij} \,, \tag{3}$$

with the Kronecker delta δ_{ij} equal to 1 for i=j, and 0 otherwise. Such a system of unit vectors is referred to as an *orthonormal basis* for a vector, which means that each vector can be represented as a linear combination of basis vectors, and the coordinates of any vector \mathbf{x} can be extracted via projection onto the corresponding unit vector,

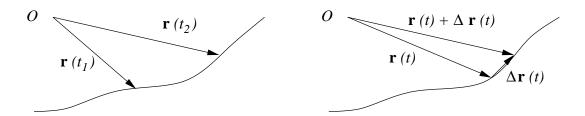
$$x_i = \mathbf{x} \cdot \mathbf{e}_i \,, \tag{4}$$

where the notation $(_\cdot_)$ denotes again the scalar product between two vectors.

An interesting property of a trajectory of a single point that moves in time according to $\mathbf{r}(t)$ is its rate of change of the position, or its velocity. This is simply the derivation of $\mathbf{r}(t)$ with respect to time,

$$\mathbf{v}(t) = \lim_{\Delta t \to 0} \frac{\mathbf{r}(t_1) - \mathbf{r}(t_2)}{\Delta t} = \frac{d\mathbf{r}(t)}{dt},$$
 (5)

with the position at two different times t_1, t_2 with a time difference $\Delta t = t_2 - t_1$ and $\Delta \mathbf{r} = \mathbf{r}(t_1) - \mathbf{r}(t_2)$ according to the following figure:



The velocity as a derivative with respect to time is often written as $\mathbf{v} = \dot{\mathbf{r}}$, and can be expressed as a linear combination of coordinate base vectors with time dependent components $v_i(t)$ with i = 1, 2, 3

$$\mathbf{v} = \sum_{i=1}^{3} v_i(t) \, \mathbf{e}_i = \sum_{i=1}^{3} \dot{r}_i(t) \, \mathbf{e}_i \,. \tag{6}$$

As can be see from the figure, the direction of the velocity vector \mathbf{v} is tangential to the trajectory in each point. Its modulus $v(t) = ||\mathbf{v}(t)||$ is referred to as the *speed* of the point, and is obtained in the usual way via the norm of the velocity vector,

$$v = ||\mathbf{v}|| = \sqrt{\mathbf{v} \cdot \mathbf{v}} = \sqrt{v_1^2 + v_2^2 + v_3^2} = \sqrt{\sum_{i=1}^3 v_i^2}.$$
 (7)

Apart from the parameterization of a trajectory with respect to time t, it is often useful to parameterize it according to its path length s. This makes it possible to describe geometrical properties of the trajectory independently of the speed with which a point may follow it. For example, we can express the velocity of a point via

$$\mathbf{v} = \lim_{\Delta s \to 0} \frac{\Delta \mathbf{r}}{\Delta s} \lim_{\Delta t \to 0} \frac{\Delta s}{\Delta t} = \frac{d\mathbf{r}}{ds} \frac{ds}{dt}.$$
 (8)

The derivative ds/dt is by definition the speed of a point, i.e., the path length increase per unit of time. This means that we can write the velocity vector as

$$\mathbf{v} = v \cdot \frac{d\mathbf{r}}{ds} =: v \cdot \mathbf{e}_t \,, \tag{9}$$

where $\mathbf{e}_t = d\mathbf{r}/ds$ is a tangential vector \mathbf{e}_t to the trajectory. Contrary to \mathbf{v} , it is a unit vector, as it can be seen by comparing (6) and (7). The transition to a parameterization of the trajectory by its path length s therefore allows a definition of a tangential vector that only depends on the geometry of the trajectory.

We now move on to another vectorial quantity, the rate of change of velocity, or the *acceleration*. This is simply the temporal derivative of the velocity,

$$\mathbf{a} = \frac{d\mathbf{v}}{dt} = \dot{\mathbf{v}} = \ddot{\mathbf{r}} \tag{10}$$

Apart from just specifying a time dependence of the Cartesian coordinates similar to (6), we can express it as a linear combination of vectors that are associated

with the trajectory. We start from (9), and apply the rule for deriving a product or two quantities:

$$\mathbf{a} = \frac{d}{dt}(v\,\mathbf{e}_t) = \frac{dv}{dt}\,\mathbf{e}_t + v\frac{d\mathbf{e}_t}{dt} = \dot{v}\,\mathbf{e}_t + v\,\frac{d\mathbf{e}_t}{dt}.$$
 (11)

The first component in this sum is pointing in the tangential direction, and, as its vectorial component \mathbf{e}_t is a unit vector, the quantity \dot{v} describes the change of velocity over time along the path. The second component in this expression contains a temporal derivative of the tangential unit vector \mathbf{e}_t . If we take the normalization condition for \mathbf{e}_t ,

$$\mathbf{e}_t \cdot \mathbf{e}_t = 1, \tag{12}$$

and derive the whole equation with respect to time, we obtain

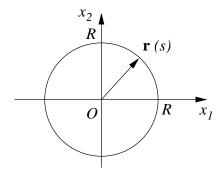
$$\frac{d}{dt}\left(\mathbf{e}_{t}\cdot\mathbf{e}_{t}\right) = \frac{d\mathbf{e}_{t}}{dt}\cdot\mathbf{e}_{t} + \mathbf{e}_{t}\cdot\frac{d\mathbf{e}_{t}}{dt} = 2\mathbf{e}_{t}\cdot\frac{d\mathbf{e}_{t}}{dt} = 0. \tag{13}$$

The vanishing dot product between product between \mathbf{e}_t and $d\mathbf{e}_t/dt$ means that the latter is a vector that is perpendicular to the tangential vector, and thus points in a direction orthogonal to the trajectory in each point. We now split up $d\mathbf{e}_t/dt$ into a modulus and a direction, and formulate it as much as we can by elements that only depends on the geometry of the trajectory. For this, we write

$$\frac{d\mathbf{e}_t}{dt} = \frac{d\mathbf{e}_t}{ds} \frac{ds}{dt} = v \left| \frac{d\mathbf{e}_t}{ds} \right| \mathbf{e}_n, \tag{14}$$

where \mathbf{e}_n is a new unit vector in the direction of the derivative of the tangent vector \mathbf{e}_t with respect to the path length. The last two factors in this expression do not contain any explicit time dependence anymore, and are thus only a property of the trajectory's geometry.

To interpret the meaning of this product, we consider a circular trajectory parameterized by s, with



$$\mathbf{r}(s) = R \left[\cos \left(\frac{s}{R} \right) \mathbf{e}_1 + \sin \left(\frac{s}{R} \right) \mathbf{e}_2 \right]$$
 (15)

By taking the derivative with respect to s, one finds

$$\frac{d\mathbf{r}}{ds} = R \left[-\sin\left(\frac{s}{R}\right) \frac{1}{R} \mathbf{e}_1 + \cos\left(\frac{s}{R}\right) \frac{1}{R} \mathbf{e}_2 \right] = -\sin\frac{s}{R} \mathbf{e}_1 + \cos\frac{s}{R} \mathbf{e}_2, \quad (16)$$

making use of several derivation rules, and the fact that the unit vectors $\mathbf{e}_{1,2}$ do not depend on s. The derivative $d\mathbf{r}/ds$ has the norm 1 because of $\sin^2(s/R) + \cos^2(s/R) = 1$, and is thus the unit tangential vector \mathbf{e}_t to the trajectory (15), i.e., $d\mathbf{r}/ds = \mathbf{e}_t$. We now proceed to take the next derivative with respect to s:

$$\frac{d\mathbf{e}_t}{ds} = -\frac{1}{R}\cos\frac{s}{R}\,\mathbf{e}_1 - \frac{1}{R}\sin\frac{s}{R}\,\mathbf{e}_2 = -\frac{1}{R}\left(\cos\frac{s}{R}\,\mathbf{e}_1 + \sin\frac{s}{R}\,\mathbf{e}_2\right) \tag{17}$$

The term in the parenthesis is again a unit vector, which we denote \mathbf{e}_n , as it is normal to \mathbf{e}_t . Thus, the derivative

$$\frac{d\mathbf{e}_t}{ds} = -\frac{1}{R}\,\mathbf{e}_n\tag{18}$$

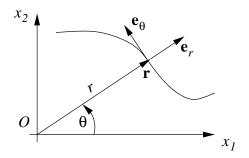
for this circular trajectory has a modulus that is inversely proportional to the radius R of the circle. As any (reasonably smooth) trajectory can locally be approximated by an arc of a circular trajectory, we now can identify the last two terms in (14) with a local radius of curvature R. With this and (14) we can write the expression (11) for the acceleration as

$$\mathbf{a} = \dot{v}\,\mathbf{e}_t + v^2\,\frac{1}{R}\,\mathbf{e}_n\,,\tag{19}$$

where some care has to be taken with the direction of the unit vector \mathbf{e}_n of the trajectory. The quantity 1/R is also referred to as the local *curvature* of the trajectory in any point. A straight trajectory with $d\mathbf{e}_t/ds = 0$ has curvature 0.

1.2 Vectors in polar coordinates

So far, we have chosen Cartesian coordinates to describe the trajectory of a point, and some of its derived quantities. We now try to do this (for a two-dimensional problem) in another coordinate system, the polar coordinates. The



polar coordinates (r, θ) are connected to the Cartesian counterparts (x_1, x_2) via

$$x_1 = r\cos\theta \,, \quad x_2 = r\sin\theta \tag{20}$$

While a trajectory can simply be specified by describing the coordinate pair (r, θ) as a function of a parameter like time t or path length s, the description of directed, vector-like quantities becomes more tricky. We do need a basis to describe vectors that is somehow connected to the coordinates. Such vectors can be constructed from the direction specified by the position change from a given point \mathbf{r} to $\mathbf{r}+d\mathbf{r}$ if one of the coordinates is changed, i.e., $r \to r+dr$ or $\theta \to \theta+d\theta$. From (20) we find (in Cartesian coordinates)

$$\mathbf{e}_{r} = const_{1} \cdot \frac{\partial}{\partial r} (x_{1} \mathbf{e}_{1} + x_{2} \mathbf{e}_{2}) = \cos \theta \mathbf{e}_{1} + \sin \theta \mathbf{e}_{2}$$

$$\mathbf{e}_{\theta} = const_{2} \cdot \frac{\partial}{\partial \theta} (x_{1} \mathbf{e}_{1} + x_{2} \mathbf{e}_{2}) = -\sin \theta \mathbf{e}_{1} + \cos \theta \mathbf{e}_{2}, \qquad (21)$$

where the constants are chosen to normalize the vectors. In the first equation, this constant is 1, in the second equation it is 1/r. Both vectors \mathbf{e}_r , \mathbf{e}_θ form an orthonormal basis, that can be used to express vectors anywhere in (here: two dimensional) space.

As an example, we now express velocity and acceleration vectors of a moving point in these coordinates. First, we note that any point in the trajectory $\mathbf{r}(t)$ can be expressed as

$$\mathbf{r} = r \,\mathbf{e}_r \tag{22}$$

We then arrive at the velocity by taking the temporal derivative:

$$\mathbf{v} = \frac{d}{dt} (r \, \mathbf{e}_r) = \dot{r} \, \mathbf{e}_r + r \, \frac{d\mathbf{e}_r}{dt}$$
 (23)

We use the product rule to carry out the differentiation, because \mathbf{e}_r will depend on the position of the point, and may thus not be constant over time. As we are looking for changes of \mathbf{e}_r , we can attempt to look for changes in the new coordinates:

$$\frac{d\mathbf{e}_r}{dt} = \frac{\partial \mathbf{e}_r}{\partial \theta} \frac{d\theta}{dt} + \underbrace{\frac{\partial \mathbf{e}_r}{\partial r}}_{=0} \frac{dr}{dt} = \mathbf{e}_\theta \frac{d\theta}{dt} = \dot{\theta} \, \mathbf{e}_\theta$$
 (24)

With this, we can write the velocity vector as a linear combination of the new unit vectors $\mathbf{e}_r, \mathbf{e}_\theta$:

$$\mathbf{v} = \dot{r}\,\mathbf{e}_r + r\dot{\theta}\,\mathbf{e}_{\theta} \tag{25}$$

Similarly, we try to express the acceleration in the basis $(\mathbf{e}_r, \mathbf{e}_\theta)$:

$$\mathbf{a} = \frac{d\mathbf{v}}{dt} = \ddot{r}\,\mathbf{e}_r + \dot{r}\,\frac{d\mathbf{e}_r}{dt} + (\dot{r}\dot{\theta} + r\ddot{\theta})\,\mathbf{e}_\theta + r\dot{\theta}\,\frac{d\mathbf{e}_\theta}{dt}$$
(26)

We obtain the temporal derivation of e_{θ} in a similar way as in (24):

$$\frac{d\mathbf{e}_{\theta}}{dt} = \frac{\partial \mathbf{e}_{\theta}}{\partial \theta} \frac{d\theta}{dt} + \underbrace{\frac{\partial \mathbf{e}_{\theta}}{\partial r}}_{=0} \frac{dr}{dt} = \dot{\theta} \frac{\partial \mathbf{e}_{\theta}}{\partial \theta} = -\dot{\theta} \,\mathbf{e}_{r} \tag{27}$$

The latter step follows from (21) by differentiation of \mathbf{e}_{θ} and comparison with \mathbf{e}_{r} . We now can clean up the expression for the acceleration, and arrive at

$$\mathbf{a} = (\ddot{r} - r\dot{\theta}^2)\,\mathbf{e}_r + (2\dot{r}\dot{\theta} + r\ddot{\theta})\,\mathbf{e}_{\theta} \tag{28}$$

The strategy how to obtain local unit vectors can be applied to other coordinate systems. It is an important method to find a basis to express vectorial quantities in whatever coordinate system is chosen.

1.3 Angular velocity

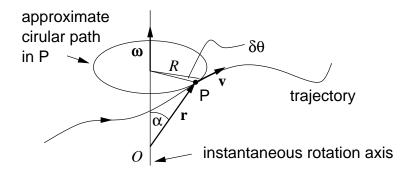
So far, we have encountered the vector quantities for the velocity \mathbf{v} , which describes the rate of change of the position \mathbf{r} of a point in time, and the acceleration \mathbf{a} , which describes the rate of changes of the velocity.

We now come back to the motion of a point on a circular trajectory defined by (15). Here, polar coordinates (r, θ) as defined in (20) simplify the description because r is constant. In a trajectory is parameterized by time t, all information about the motion is contained in the function $\theta(t)$. Similar to the linear motion, we can introduce an angular velocity ω for the instantaneous rate of change of θ :

$$\omega(t) = \frac{d}{dt}\theta(t) \tag{29}$$

This is a simple quantity for a motion in two dimensions. As any motion in three dimensions can be locally approximated by a circular arc, we look more carefully at a circular motion in three dimensions. The approximate circular motion in each point has a well-defined axis of rotation. This axis can be well described by a vector, with an ambiguity in the pointing direction (because an axis is equally well described by two vectors $\boldsymbol{\omega}$ and $-\boldsymbol{\omega}$), and its length. In the same way as the rate of change of the position is encoded in the length $v = |\mathbf{v}|$ of the velocity vector \mathbf{v} , we now encode the rate of change of the angle, $\omega = d\theta/dt$ of the approximate circular motion, into the length of a vector $\boldsymbol{\omega}$, which points in the axis of rotation. We can fix the pointing ambiguity by postulating that \mathbf{v} , $\mathbf{a} = \dot{\mathbf{v}}$ (which is perpendicular to \mathbf{v}), and $\boldsymbol{\omega}$ form a right-handed system. Note that here the angle θ refers to a polar coordinate system with an origin in the center of the approximating circle. This definition of $\boldsymbol{\omega}$ is independent of any coordinate system, a property that seems sensible to postulate for meaningful physical quantities.

We now check the relation between \mathbf{v} , \mathbf{r} and $\boldsymbol{\omega}$ if we choose a coordinate system that has an origin somewhere on the axis of the rotation as shown in the figure.



The modulus of the velocity is given by $v = \omega R = \omega |\mathbf{r}| \sin \alpha$, and \mathbf{v} is perpendicular both on \mathbf{r} and $\boldsymbol{\omega}$. This relationship is fulfilled by the vector product

$$\mathbf{v} = \boldsymbol{\omega} \times \mathbf{r} \,, \tag{30}$$

which incidentally also matches the choice for the direction of ω .

In analogy to the velocity \mathbf{v} describing the rate of change of a position in space \mathbf{r} , and the simple relation $\mathbf{v} = \dot{\mathbf{r}}$, this may suggest that there is a vector quantity that has the meaning of an angle, and its temporal derivative leads to the vector quantity $\boldsymbol{\omega}$ above. This, however, will not work. To see why, we need to have a closer look to coordinate transformations.

1.4 Coordinate transformations

It can be useful to describe a vector quantity like the velocity in different coordinate systems. The usual Cartesian coordinate system with some origin is one of them, the tangential coordinate system to a trajectory, defined by \mathbf{e}_t from (9), \mathbf{e}_n from (11) and a third unit vector, $\mathbf{e}_r = \mathbf{e}_t \times \mathbf{e}_n$ orthogonal to the first two, is another one. Yet other Cartesian reference frames can be generated from tangential vectors to polar, spherical or cylindrical coordinate systems. They all have the property that any vector can be expressed as a linear combination of the respective basis vectors:

$$\mathbf{a} = \sum_{i=1}^{3} a_i \mathbf{e}_i \tag{31}$$

Any transition from a right-handed basis $\{e_1, e_2, e_3\}$ to a different right-handed basis $\{e'_1, e'_2, e'_3\}$ can be expressed as a rotation in space. This can be shown rigorously, but we skip this here and refer to a course in basic linear algebra. The coordinate transformation should not affect the scalar product of two vectors, and as a consequence, norm of a single vector should be conserved, i.e,

$$\mathbf{a}' \cdot \mathbf{b}' = \sum_{i=1}^{3} a'_i b'_i = \sum_{i=1}^{3} a_i b_i = \mathbf{a} \cdot \mathbf{b}, \qquad (32)$$

with components a_i and a'_i in the respective bases. The transformation between the coordinates is a linear relationship, and can be represented by

$$\begin{pmatrix} a'_{1} \\ a'_{2} \\ a'_{3} \end{pmatrix} = \mathbf{M} \cdot \begin{pmatrix} a_{1} \\ a_{2} \\ a_{3} \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{pmatrix} \cdot \begin{pmatrix} a_{1} \\ a_{2} \\ a_{3} \end{pmatrix} \quad \text{or} \quad a'_{i} = \sum_{j=1}^{3} m_{ij} a_{j} ,$$

$$(33)$$

with the matrix \mathbf{M} made up by components m_{ij} . The matrix representation \mathbf{M} of a linear transformation that preserves the scalar product between two vectors obeys $|\det \mathbf{M}| = 1$.

We now look at specific examples for rotations and their representation in the form (33). A rotation around the \mathbf{e}_3 axis by an angle ϕ is represented by

$$\mathbf{R}_3(\phi) = \begin{pmatrix} \cos \phi & -\sin \phi & 0\\ \sin \phi & \cos \phi & 0\\ 0 & 0 & 1 \end{pmatrix} \tag{34}$$

Matrix representations of rotations around axes $\mathbf{e}_{1,2}$ can be obtained by cyclic coordinate change $1 \to 2 \to 3 \to 1$ (or $x \to y \to z \to x$):

$$\mathbf{R}_{1}(\phi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & -\sin\phi \\ 0 & \sin\phi & \cos\phi \end{pmatrix} \quad \text{and} \quad \mathbf{R}_{2}(\phi) = \begin{pmatrix} \cos\phi & 0 & \sin\phi \\ 0 & 1 & 0 \\ -\sin\phi & 0 & \cos\phi \end{pmatrix} \quad (35)$$

Rotations around different axes do generally not commute. The matrix representing two sequential transformations is the matrix product of the representations of the individual transformations. For example,

$$\mathbf{R}_{2}(90^{\circ}) \cdot \mathbf{R}_{3}(90^{\circ}) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad (36)$$

but

$$\mathbf{R}_{3}(90^{\circ}) \cdot \mathbf{R}_{2}(90^{\circ}) = \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{pmatrix} \neq \mathbf{R}_{2}(90^{\circ}) \cdot \mathbf{R}_{3}(90^{\circ}).$$
 (37)

If we were to represent a rotation by a vector, the sum of two such vectors would be again a vector representing a rotation that should represent the concatenation of the rotations represented by the individual vectors; this can be motivated by looking at two rotations around the same axis. For different axes, however, the representation of concatenated rotations depend on their sequence, but the sum of two vectors does not. Hence, a rotation by a finite angle can not be represented in a meaningful way by a vector. This answers, in part, the problem we were facing at the end of section 1.3: there is no underlying vector quantity which has the angular velocity vector ω as a rate of change in time.

We stay for a while with the properties of rotation transformations. They are still meaningful independently of the choice of a coordinate system, although they can not represented by vectors. Specifically, observers with different coordinate systems can agree on a rotation axis, direction, and angle.

As rotations can be represented by matrices that transform vectors according to (33), and such matrices can again be represented in different coordinate systems, we can try to extract properties of rotation transformations that are independent of the coordinate system. The determinant det M of a representing matrix M is such a property. Others are the eigenvalues of a representing matrix. For the specific example of a rotation around e_3 in (34), we can evaluate the characteristic equation to determine the eigenvalues λ :

$$|\mathbf{R}_{3}(\phi) - \lambda \mathbf{I}| = \begin{vmatrix} c - \lambda & -s & 0 \\ s & c - \lambda & 0 \\ 0 & 0 & 1 - \lambda \end{vmatrix} = (1 - \lambda)[(c - \lambda)^{2} + s^{2}] = 0, \quad (38)$$

with $c = \cos \phi$, and $s = \sin \phi$. This can be further simplified to

$$(1 - \lambda)(1 - 2c\lambda + \lambda^2) = 0. \tag{39}$$

The first eigenvalue is $\lambda = 1$; one corresponding eigenvector is

$$\mathbf{a} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \mathbf{e}_3. \tag{40}$$

This represents the fact that vectors along the rotation axis do not change. More generally, an eigenvector to the eigenvalue 1 of a matrix representing an arbitrary rotation provides a nice way to find the axis of rotation in any Cartesian coordinate system. For the other two eigenvalues λ that fulfill (39), we find the roots to the second factor $(1 - 2\cos\phi\lambda + \lambda^2)$:

$$\lambda = \cos \phi \pm \sqrt{\cos^2 \phi - 1} = \cos \phi \pm \sqrt{-1}\sqrt{1 - \cos^2 \phi}$$
$$= \cos \phi \pm i \sin \phi = e^{\pm i\phi}$$
(41)

Therefore, we can extract the angle of rotation represented by a matrix by looking at its complex eigenvalues. As a side remark, the corresponding eigenvectors for a rotation represented by $\mathbf{R}_3(\phi)$ are $\mathbf{a} = \mathbf{e}_1 \pm i\mathbf{e}_2$. These vectors are not too meaningful in classical mechanics, but become useful e.g. when considering representations of electromagnetic fields of circular polarization; left- and right-handed polarized fields propagating along the \mathbf{e}_3 axis are represented by these eigenvectors, and are preserved under rotations around \mathbf{e}_3 .

The rotations we have considered so far all preserve the handedness of a coordinate system; they fall into the category with det $\mathbf{R} = +1$; they are so-called *proper*

rotations. Scalar-product preserving coordinate transformations with det $\mathbf{R} = -1$ are referred to as *improper rotations*, and are are concatenations of (an odd number of) coordinate inversions, or mirror images with proper rotations. For example, a reflection in direction of \mathbf{e}_3 is represented by the matrix

$$\mathbf{M}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} . \tag{42}$$

We have seen examples of vectors like velocity and acceleration. For a change to a different orthogonal coordinate system, they need to be transformed according to (33). Physical quantities like temperature in a given location or the speed of a point that do not change under coordinate changes form the class of scalars. We can extend this concept and ask e.g. how to transform the representations of physical properties that need to be represented by matrices. Such quantities, apart from the rotations we just saw, do exist; an example in continuum mechanics would be the stress tensor), but this is beyond the scope of this module. The moment of inertia of a solid is another one. If such a quantity (referred to as tensor of rank 2) is represented by a matrix \mathbf{T} made up by components t_{ij} , its components transform under \mathbf{M} according to

$$t'_{ij} = \sum_{k,l=1}^{3} m_{ik} m_{jl} t_{kl} \tag{43}$$

One can turn these transformation properties around, and classify a physical property as scalar, vector or tensor according to their transformation properties: Scalars do not change under rotations, vector are transformed according to (33), tensors of rank 2 according to (43), and so on.

1.5 Infinitesimal rotations

Examples (36) and (37) show that finite rotations generally do not commute. However, the situation changes if we consider only small rotations. Starting from (30), we find a change of a position \mathbf{r} in a small time interval δt :

$$\mathbf{r} \to \mathbf{r} + \delta \mathbf{r}_1$$
 with $\delta \mathbf{r}_1 = \mathbf{v} \delta t = (\boldsymbol{\omega} \delta t) \times \mathbf{r} = \delta \boldsymbol{\theta}_1 \times \mathbf{r}$, (44)

where $\delta \boldsymbol{\theta}_1$ represents a small rotation by an angle $\delta \boldsymbol{\theta}_1$ around an axis parallel to $\delta \boldsymbol{\theta}_1$, and a handedness in the same way as defined for $\boldsymbol{\omega}$.

Two sequential infinitesimal rotations, $\delta \theta_1$ followed by $\delta \theta_2$, change the position \mathbf{r} of a point similarly to (44) by the infinitesimal amount

$$\delta \mathbf{r}_{12} = \delta \mathbf{r}_1 + \delta \boldsymbol{\theta}_2 \times (\mathbf{r} + \delta \mathbf{r}_1)
= \delta \boldsymbol{\theta}_1 \times \mathbf{r} + \delta \boldsymbol{\theta}_2 \times (\mathbf{r} + \delta \boldsymbol{\theta}_1 \times \mathbf{r})
= \delta \boldsymbol{\theta}_1 \times \mathbf{r} + \delta \boldsymbol{\theta}_2 \times \mathbf{r} + \delta \boldsymbol{\theta}_2 \times \delta \boldsymbol{\theta}_1 \times \mathbf{r}
\approx \delta \boldsymbol{\theta}_1 \times \mathbf{r} + \delta \boldsymbol{\theta}_2 \times \mathbf{r}$$
(45)

by neglecting the product term of two infinitesimal quantities in the last step. This representation is the same if one carries out the rotations in different order. As a consequence, infinitesimal rotations represented by vectors $\delta \theta$ do commute.

We can also see this with an infinitesimal version of our example in (36) and (37). We first approximate the representation (34) by a truncated Taylor expansion for small angles $\delta\theta$:

$$\mathbf{R}_{3}(\delta\theta_{3}) = \begin{pmatrix} 1 - \delta\theta_{3}^{2}/2 + \dots & -\delta\theta_{3} + \delta\theta_{3}^{3}/3! - \dots & 0\\ \delta\theta_{3} - \delta\theta_{3}^{3}/3! + \dots & 1 - \delta\theta_{3}^{2}/2 + \dots & 0\\ 0 & 0 & 1 \end{pmatrix} \approx \begin{pmatrix} 1 & -\delta\theta_{3} & 0\\ \delta\theta_{3} & 1 & 0\\ 0 & 0 & 1 \end{pmatrix},$$
(46)

again by neglecting terms in higher than linear order in $\delta\theta$. Similarly, we approximate $\mathbf{R}_2(\delta\theta_2)$, and evaluate two concatenated small rotation matrices. We find

$$\mathbf{R}_{2}(\delta\theta_{2}) \cdot \mathbf{R}_{3}(\delta\theta_{3}) = \begin{pmatrix} 1 & -\delta\theta_{3} & \delta\theta_{2} \\ \delta\theta_{3} & 1 & 0 \\ -\delta\theta_{2} & \delta\theta_{2}\delta\theta_{3} & 1 \end{pmatrix}$$
(47)

and

$$\mathbf{R}_{3}(\delta\theta_{2}) \cdot \mathbf{R}_{3}(\delta\theta_{3}) = \begin{pmatrix} 1 & -\delta\theta_{3} & \delta\theta_{2} \\ \delta_{3} & 1 & \underline{\delta\theta_{2}\delta\theta_{3}} \\ -\delta\theta_{2} & 0 & 1 \end{pmatrix}. \tag{48}$$

The two expressions differ only by the two underlined terms, which is a product of two infinitesimal angles. Neglecting them with the same argument used for truncating the Taylor expansion, the infinitesimal rotations commute.

So in summary, an infinitesimal rotation can be represented by a vector $\delta \boldsymbol{\theta}$. The direction of this vector characterizes the rotation axis, and can be transformed in a meaningful way according to (33). Its modulus represents the rotation angle, and the sum of two vectors $\delta \boldsymbol{\theta}_1 + \delta \boldsymbol{\theta}_2$ represents correctly the concatenation of the two individual infinitesimal rotations.

2 Newtonian Mechanics for single particles

So far, we only looked at a mathematical description of trajectories. One of the main goals in classical mechanics is to describe the evolution of a physical system in time. An extremely successful method for this was developed by Sir Isaac Newton. The idea is not to specify the whole trajectory of a particle, but to combine very few underlying universal principles with standard mathematical methods. These principles were expressed as "laws", and are sufficient (together with some initial parameters) to lead to a complete description of the evolution of a physical system.

These laws, together with the mathematical tools to solve differential equations, have turned out to be tremendously successful in the description of mechanical

systems over an extremely wide scales in space and time, ranging from motion on the molecular level up to the motion of planets. It was not until perhaps a 120 years ago that the descriptive strength of these few "laws" has been seen as incomplete for describing the motion of mechanical objects, specifically for areas where very small masses, extremely short time scales, high energies, and velocities on the order of the speed of light are involved.

That said, Newton's laws turned physics into a science with an enormous predictive power based on very few and simple rules, and cover extremely well the phenomena that we encounter in our daily life.

2.1 Newton's laws

Sir Isaac Newton formulated these laws in 1687 in his "Principia". They were formulated as follows:

- I. A body remains at rest or in uniform motion unless acted upon a force.
- II. A body acted upon a force moves in such a manner that the time rate of change of momentum equals the force.
- III. If two bodies exert forces on each other, these forces are equal in magnitude and opposite in direction.

These laws do not mean that the physical world has to follow them strictly—they are more a tool to efficiently describe how many things evolve in time. In a sufficiently well specified context of initial conditions and participating forces, they and allow a very accurate description of the motion of objects. However, it is necessary to observe how well Newton's laws (or any other physical law) capture a phenomenon in nature to see if corrections or additional principles need to be added.

When these laws were formulated, the whole mathematical language of definitions and formal logic was not as formally developed as it is now. Thus, it makes sense to comment on these laws to make clearer what they actually state.

The first law is basically a definition of a "free particle". The notion of a force is used, but not introduced in a too useful way. "Uniform motion" means that the velocity of a particle does not change in time. For making a statement about a velocity, we do require a specific reference frame, i.e., the choice of an origin and a few other properties that we will see later. Formally, we would write the first law as

$$\mathbf{F} = 0 \Rightarrow \mathbf{v} = const.$$
 (49)

The second law explicitly relates force with momentum (called *quantity of motion* originally), and Newton provided a definition of the momentum of a particle as

$$\mathbf{p} = m\mathbf{v} \,, \tag{50}$$

where m is the mass of a particle, and \mathbf{v} its velocity. Mathematically, the second law can be written as

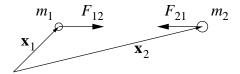
$$\mathbf{F} = \frac{d}{dt}\mathbf{p} = \frac{d}{dt}(m\mathbf{v}) = m\mathbf{a} = m\ddot{\mathbf{x}}.$$
 (51)

This is a definition of what is meant by force. However, this definition requires that one has already an idea what the mass m of an object is. While it seems intuitively clear, this is a reference to the $inertial\ mass$ of an object. It is an intrinsic quantity of an object that is not subject of its state of motion.

The third law is a statement on the motion of *two objects* that exert forces on each other. Even more specific, it makes reference to forces aligned along the connecting line between them,

$$\mathbf{F}_{12} \parallel (\mathbf{x}_1 - \mathbf{x}_2), \tag{52}$$

where \mathbf{x}_1 and \mathbf{x}_2 are the positions of the two objects. Such forces are referred to as *central forces*, but the choice of the name "central" will only become clear at a stage when we consider objects of finite size. Examples of such forces are forces exerted by a elastic spring connecting the two bodies, the gravitational force between two heavy masses, or the force between two electrically charged objects, van der Waals forces, and others.



In such a case, the third law then states that

$$\mathbf{F}_{12} = -\mathbf{F}_{21} \tag{53}$$

Notably, the third law does not apply to forces that depend on the velocity of particles. Examples for such forces are the friction of an object moving through a medium, or even the (weak) velocity dependence of the gravitational force.

Together with the definition of force in the second law in (51), one can write the third law in its version (53):

$$m_1 \frac{d\mathbf{v}_1}{dt} = -m_2 \frac{d\mathbf{v}_2}{dt}$$
 or $m_1 \mathbf{a}_1 = -m_2 \mathbf{a}_2$ or $\frac{m_1}{m_2} = -\frac{a_2}{a_1}$, (54)

where the minus sign indicates the opposite orientation of the two accelerations on the two masses. This relation can be used to compare the two inertial masses by comparing the accelerations of the two bodies when they exert a force on each other. Again, an appropriate reference frame is necessary to determine the accelerations.

We often do not measure the ratio of inertial masses, but that of heavy masses in the gravitational field of the earth with a balance. It does not follow by logic from Newton's law that the heavy mass and the inertial mass used in the definition of a force (51) are the same. However, many tests have been carried out that compared heavy and inertial masses that seem to indicate that they are indeed the same property. Often Galileo is attributed to have carried out the first of these tests by comparing the falling time of balls of the same material, but different masses from the tower of Pisa some time around 1600, but apparently Simon Stevin seemed to have actually carried out this experiment on the church tower in Delft in 1586. Those early experiments had a limited accuracy, and experiments carried out by Newton himself seemed to have shown the equivalence of heavy and inertial mass "only" to within 10^{-3} . Much more accurate tests were carried out by Eötvös¹ in 1890, and more recent experiments by Dicke² in 1964 could show the equivalence of the two quantities to within 10^{-12} . This seems to suggest that they are indeed equivalent. The assertion that the two are equivalent is referred to as the equivalence principle, and is one of the cornerstones of general theory of relativity.

Another important consequence of the third law can be seen when using the definition of the force in the form of $\mathbf{F} = d\mathbf{p}/dt$ in an isolated system of two bodies 1,2. Then, it states

$$\frac{d\mathbf{p}_1}{dt} = -\frac{d\mathbf{p}_2}{dt} \quad \text{or} \quad \frac{d}{dt}(\mathbf{p}_1 + \mathbf{p}_2) = 0.$$
 (55)

This means that the sum $\mathbf{p}_1 + \mathbf{p}_2$ of the two momenta is constant in time, i.e., the total momentum in this system is *conserved*. We will see a few more of such conservation laws, they tend to simplify the description of the dynamics of a system.

2.2 Inertial reference frames

The consequences of Newton's laws only make sense if there is an appropriate coordinate system that is used to describe the derivatives of the momentum via (53). Such coordinate systems are referred to as *inertial reference frames*. Therefore, a somewhat lame definition of such a reference system is can be seen as one in which Newton's laws hold. Then, the first law (49) can be used as a definition: An *inertial reference frame* is a reference frame in which a body under no influence of a force remains in uniform motion.

Once one has identified an inertial reference frame, there are several others: As Newton's laws make statements about the *change* of velocities of bodies, the addition of a constant velocity does not affect the validity of the laws. Thus,

¹Loránd Eötvös, 1848-1919

²Robert H. Dicke, 1916-1997

a coordinate transformation between two reference systems K and K' with a position vector of a point \mathbf{r} in K, and \mathbf{r}' in K' according to

$$\mathbf{r} \to \mathbf{r}' = \mathbf{r} + \mathbf{v}_0 t \tag{56}$$

with a constant velocity \mathbf{v}_0 leads to $\ddot{\mathbf{r}} = \ddot{\mathbf{r}}'$. Thus, if Newton's laws hold in K, they also do in K'. It should be noted that the times t and t' in the two reference systems are assumed to be the same. Such transformations are referred to as *Galilean transformations*, the equivalence of two inertial frames under such a transformation is referred to as *Galilean invariance*, or the principle of *Newtonian or Galilean relativity*.

2.3 Equation of motion

We can now use Newton's second law (51) to determine the dynamic of a system, simply by considering

$$\mathbf{F} = m\ddot{\mathbf{x}} \tag{57}$$

as a differential equation for the position \mathbf{x} of a body. This is a second order ordinary differential equation (ODE), which we can solve if we know the force \mathbf{F} acting on the body, and sufficient initial or boundary conditions for the position and/or velocities. However, this equation of motion does not always hold. Examples where this is *not* applicable are

- situations in non-inertial reference frames, like rotating reference frames. This becomes significant e.g. in the description of the motion of air particles and clouds on long ranges;
- at velocities that are not small compared to the speed of light;
- when time would be not homogenous. This is perhaps a rather exotic restriction.

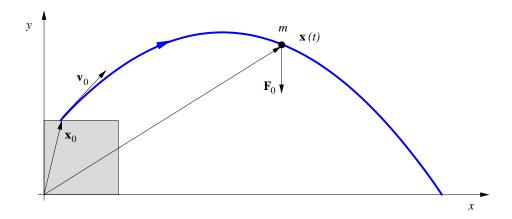
2.3.1 Free Fall

A simple equation of motion is presented for a constant force $\mathbf{F} = \mathbf{F}_0$. Then, the acceleration $\mathbf{a} = \mathbf{F}_0/m$ is constant as well, and we can obtain the velocity by integration over time:

$$\mathbf{v}(t) = \int_{0}^{t} \mathbf{a}(t')dt' + \mathbf{v}_{0} = \frac{1}{m}\mathbf{F}_{0}t + \mathbf{v}_{0}, \qquad (58)$$

where \mathbf{v}_0 is the velocity of the particle at time t = 0. The position $\mathbf{x}(t)$ of the particle at any time t follows from integration of $\mathbf{v}(t)$,

$$\mathbf{x}(t) = \int_{0}^{t} \mathbf{v}(t')dt' + \mathbf{x}_{0} = \frac{1}{2m}\mathbf{F}_{0}t^{2} + \mathbf{v}_{0}t + \mathbf{x}_{0}, \qquad (59)$$



With the additional integration constant \mathbf{x}_0 fixing the position at t = 0. A typical example for such a case is the acceleration of a body with a mass m under the influence of gravity on earth, ignoring eventual friction forces. Such a motion is called *free fall*, but can have initial conditions that include a velocity component that points in an arbitrary direction.

This is a nice example where one can see that the vectorial equation of motion (and its solution) separates into individual components. In the example shown in the figure, the constant force \mathbf{F}_0 has no component in x direction. Therefore, the motion in x is uniform, i.e., the velocity component v_x is constant, and the component x(t) increases linearly in time. For the component in y, the motion is quadratic in t. The choice of a suitable coordinate system therefore can simplify the integration of the equation of motion, and separate out certain degrees of freedom.

2.3.2 Friction Forces

Another class of forces are friction forces. They appear when an object moves in a fluid, or in contact with a surface, and opposes the motion of a particle. They depend on the velocity either linearly,

$$\mathbf{F} = -\alpha \mathbf{v} \tag{60}$$

with a positive constant α , or more generally,

$$\mathbf{F} = -f(v)\frac{\mathbf{v}}{v} \tag{61}$$

with a function f(v) depending on the speed v of the object. The dependency can be rather complex and depends on the nature of the friction, and on the velocity range. If something moves through a fluid like air slow enough, $f(v) \propto v$ as in (60), but for higher speeds, a quadratic dependency is observed. An approximate heuristic formulation of such a friction force that is used to describe the drag of

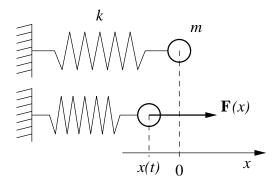
objects like cars or bicycles moving through air is

$$f(v) = \frac{1}{2}c_W \rho A v^2, \qquad (62)$$

with the density of air ρ , the surface A area of the vehicle, and a dimensionless shape-dependent drag coefficient c_W that is around 0.3 for most cars these days, and around 1 for someone on a bicycle for typical speed ranges. If v comes close to the speed of sound, f(v) undergoes a relatively complex change.

2.3.3 Harmonic oscillator

The motion of a harmonic oscillator is a particularly important and appears in many areas of physics. We consider the simple case where a mass m is connected to a spring with a Hook constant k, and motion only takes place in x direction:



The spring exerts a restoring force F_x on the mass,

$$F_x = -kx\,, (63)$$

and with (51) or $F_x = m\ddot{x} = -kx$, the equation of motion takes the form

$$\ddot{x}(t) + \frac{k}{m}x(t) = 0. \tag{64}$$

This is a linear ordinary differential equation, because all derivatives of x appear linearly. Such equations have special solutions

$$x(t) = e^{st} (65)$$

with a (generally complex) constant s. Inserting (65) into (64) leads to

$$\left(s^2 + \frac{k}{m}\right)x(t) = 0.$$
(66)

As this equation has to hold for all times, the first term needs to vanish:

$$s^2 + \frac{k}{m} = 0 \tag{67}$$

This is referred to as the characteristic equation of (64). Its two roots are

$$s_{1,2} = \pm \sqrt{-\frac{k}{m}} = \pm i\sqrt{\frac{k}{m}} = \pm i\omega \quad \text{with} \quad \omega = \sqrt{\frac{k}{m}}$$
 (68)

Because the roots $s_{1,2}$ are distinct, the general solution of (64) is a linear combination of the two solutions (65) for s_1 and s_2 ,

$$x(t) = a_1 e^{s_1 t} + a_2 e^{s_2 t} = a_1 e^{i\omega t} + a_2 e^{-i\omega t}.$$
 (69)

The constants $a_{1,2}$ are now chosen to meet the initial conditions of the differential equation. To fully determine the motion in time, exactly two initial conditions are needed; let's assume $x(t=0) = x_0$, and $v(t=0) = \dot{x}(t=0) = 0$. Inserting these conditions into (69) leads to

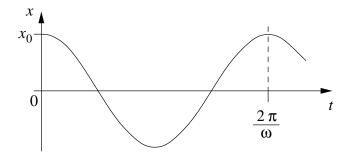
$$x(t=0) = a_1 + a_2 = x_0 (70)$$

$$\dot{x}(t=0) = a_1 i\omega - a_2 i\omega = i\omega(a_1 - a_2) = 0 \tag{71}$$

The second part leads to $a_1 = a_2$, and the first part then to $a_1 = x_0/2$, so we finally get the oscillatory solution to (64) that meets the initial conditions,

$$x(t) = \frac{x_0}{2} \left(e^{i\omega t} + e^{-i\omega t} \right) = x_0 \cos \omega t , \qquad (72)$$

with the oscillatory solution of amplitude x_0 and a period $2\pi/\omega$:

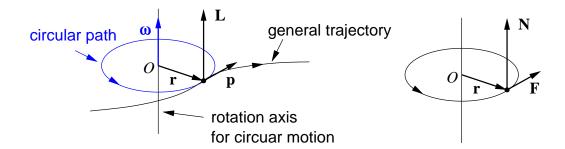


2.4 Angular motion

Newton's laws introduce the concept of momentum, which is changed by a force, and can be used to make a statement about the linear motion of a body. If no force is acting on the body, the linear momentum \mathbf{p} is conserved. Similarly for angular motion, one can formally define a vector termed angular momentum \mathbf{L} :

$$\mathbf{L} := \mathbf{r} \times \mathbf{p} \,, \tag{73}$$

where \mathbf{r} is the position of a particle with respect to some origin O, and $\mathbf{p} = m\mathbf{v}$ its linear momentum. This definition does not imply any circular motion, but it is



inspired by it, as shown below: In the case of a circular trajectory and a constant speed v, the newly defined vector \mathbf{L} is constant, and points in the direction of the earlier introduced angular velocity $\boldsymbol{\omega}$.

The temporal derivative of the angular momentum defined in (73) is given by:

$$\dot{\mathbf{L}} = \frac{d}{dt} (\mathbf{r} \times \mathbf{p})
= \dot{\mathbf{r}} \times \mathbf{p} + \mathbf{r} \times \dot{\mathbf{p}}
= \underbrace{\mathbf{v} \times (m\mathbf{v})}_{=0} + \mathbf{r} \times \dot{\mathbf{p}}
= \mathbf{r} \times \mathbf{F},$$
(74)

where \mathbf{F} is the force acting on the particle. Similar to the definition of \mathbf{L} in (73), one can define a vector \mathbf{N} called *torque* with respect to an origin O:

$$\mathbf{N} := \mathbf{r} \times \mathbf{F} \tag{76}$$

With this definition, the temporal derivative of L is simply given by

$$\dot{\mathbf{L}} = \mathbf{N} \tag{77}$$

This looks similar to the second law for linear momentum, $\dot{\mathbf{p}} = \mathbf{F}$, but for rotations. Thus, for angular motion, angular momentum \mathbf{L} and torque \mathbf{N} play similar roles as momentum \mathbf{p} and force \mathbf{F} for linear motion.

If $\mathbf{N} = 0$, $\mathbf{L} = 0$, i.e., the angular momentum \mathbf{L} remains constant or is conserved. An important example for this situation can be found with central force problems, like the Coulomb interaction or gravitational attraction between two heavy bodies. If the origin O for determining the angular momentum is chosen in one of the two bodies, or somewhere on the connecting line between them, the force \mathbf{F} exerted by each body to the other one is parallel to \mathbf{r} . Then,

$$\mathbf{N} = \mathbf{r} \times \mathbf{F} = \mathbf{r} \times (const \cdot \mathbf{r}) = 0. \tag{78}$$

Consequently, the angular momentum does not change in time: isolated systems governed by a central force (planets around a central star, electrons around a proton) conserve the angular momentum. This does not mean, however, that the trajectories have to be circular!

3 Work and Energy

While Newton's laws allow for a straightforward formulation of equations of motion via forces, they require a knowledge of the vectorial quantity force. This can become a bit complicated, especially if forces need to be introduced to fulfill boundary conditions and constraints. Sometimes a quantity of interest may not require to fully solve the equations of motion. On the other hand, some of the expressions for forces can get simpler as well with the introduction of concepts of work and energy. They will also be required for deriving the equations of motion of a physical system in different ways than using Newton's laws.

3.1 Kinetic energy

We start with the definition of an integral quantity between two positions 1 and 2 of a particle along a path Γ as indicated:

$$W_{12} := \int_{\Gamma_{1\to 2}} \mathbf{F} \cdot d\mathbf{s}$$

$$1 \qquad \qquad \mathbf{f} \qquad \qquad \mathbf{2}$$

$$\mathbf{ds} \qquad \qquad (79)$$

This is definition of "work" W_{12} for a transition between two points integrates up the scalar products between a local force \mathbf{F} and line elements $d\mathbf{s}$ along the path Γ . It can be evaluated component-wise,

$$\int_{\Gamma} \mathbf{F} \cdot d\mathbf{s} = \int_{\Gamma} \sum_{i} F_{i} dx_{i} \tag{80}$$

Often one can also evaluate the kernel $\mathbf{F}d\mathbf{s}$ of this integral with respect to a sensible parameterization of the path Γ , like the path length s introduced earlier,

$$\mathbf{F} \cdot d\mathbf{s} = \mathbf{F} \cdot \mathbf{e}_t \, ds \,, \tag{81}$$

where \mathbf{e}_t is the tangential vector to the path, and $d\mathbf{s}$ a length element. With $\mathbf{F} = m\dot{\mathbf{v}}$, and parameterizing via time, $d\mathbf{s} = \mathbf{v}dt$, it becomes

$$\mathbf{F} \cdot d\mathbf{s} = (m\dot{\mathbf{v}}) \cdot (\mathbf{v} dt)$$

$$= \frac{1}{2} m (2\mathbf{v}\dot{\mathbf{v}} dt)$$

$$= \frac{1}{2} m d (\mathbf{v} \cdot \mathbf{v}) = d \left(\frac{1}{2} m \mathbf{v}^{2}\right)$$
(82)

The third step in the development above can be seen as reversing the differentiation of the scalar product $\mathbf{v} \cdot \mathbf{v} =: \mathbf{v}^2$ with respect to time:

$$\frac{d}{dt}(\mathbf{v} \cdot \mathbf{v}) = \mathbf{v} \cdot \dot{\mathbf{v}} + \dot{\mathbf{v}} \cdot \mathbf{v} = 2\mathbf{v}\dot{\mathbf{v}}$$
(83)

The last step in (82) is just combining the constants into a single differential $d(m\mathbf{v}^2/2)$. By defining a quantity

$$T := \frac{1}{2}m\mathbf{v}^2\,,\tag{84}$$

one can simplify the differential $d(m\mathbf{v}^2/2) = dT$, and the work integral becomes

$$W_{12} = \int_{\Gamma_{1\to 2}} \mathbf{F} \cdot d\mathbf{s} = \int_{\Gamma_{1\to 2}} dT = T_2 - T_1$$
 (85)

This is a somewhat tricky step: by showing that $\mathbf{F} \cdot d\mathbf{s}$ can be written as a full differential dT in the newly defined quantity T, the integration becomes trivial, and the result is the difference between the two values of T at points 1 and 2.

The quantity T only depends on the velocity \mathbf{v} in a given point; it is therefore reasonable to call the definition (84) kinetic energy T of a particle. According to (85), the work W_{12} along a path Γ evaluates the change in the kinetic energy of the particle moving from point 1 to 2.

This statement holds independently of the form of the force, which can depend on the position and velocity of the particle, and explicitly on time: $\mathbf{F} = \mathbf{F}(\mathbf{r}, \mathbf{v}, t)$.

Also note that definition (84) is reasonable in the sense that T = 0 for $\mathbf{v} = 0$, but not unique: we could have chosen to add a constant T_0 to T. Such an additive constant leaves both the full differential dT unchanged, and cancels out in the subtraction (85). This is something to pay attention to whenever some quantity (here: T) is defined that conveniently describes differential property (here: $dT = \mathbf{F} \cdot d\mathbf{s}$).

3.2 Conservative forces and potential energy

For forces that only depend on the position \mathbf{r} of a particle, one can assign a "field" $\mathbf{F}(\mathbf{r})$. The work integral (79)

$$W_{12} = \int_{\Gamma_{1\to 2}} \mathbf{F}(\mathbf{r}) \cdot d\mathbf{s} \tag{86}$$

can be more directly evaluated with results from vector calculus. In some cases, the work does not even depend on the specific path Γ a particle takes, but only on the end points 1 and 2. In such cases, $\mathbf{F}(\mathbf{r})$ is called a *conservative* force.



A path integral between points 1 to 2 along a path Γ can be split up in an integral between points 1 and an intermediate point 3, and one between points 3

and 2:

If the path integral is independent of the path Γ , and therefore any intermediate point 3 like in the path above, it has to take the form of a difference of an endpoint-dependent function:

$$\int_{\Gamma_{1\to 2}} \mathbf{F} \cdot d\mathbf{s} = U(\mathbf{r}_1) - U(\mathbf{r}_2)$$
(88)

This form suggests that the integral kernel can be written as a full differential, $\mathbf{F} \cdot d\mathbf{s} = -dU$. With the ansatz

$$\mathbf{F} = -\nabla U = \sum_{i} \frac{dU}{dx_i} \mathbf{e}_i \,, \tag{89}$$

one can verify that the path integral takes indeed the form (88):

$$\int_{\Gamma_{1\to 2}} \mathbf{F} \cdot d\mathbf{s} = -\int_{\Gamma_{1\to 2}} (\nabla U) \cdot d\mathbf{s}$$

$$= -\int_{\Gamma_{1\to 2}} \left(\sum_{i} \frac{\partial U}{\partial x_{i}} \mathbf{e}_{i} \right) \left(\sum_{j} \mathbf{e}_{j} dx_{j} \right)$$

$$= -\int_{\Gamma_{1\to 2}} \sum_{i} \frac{\partial U}{\partial x_{i}} dx_{i} = -\int_{\Gamma_{1\to 2}} dU$$

$$= U(\mathbf{r}_{1}) - U(\mathbf{r}_{2}) \tag{90}$$

Similarly to the definition of the kinetic energy, the function $U(\mathbf{r})$ is not uniquely defined. By adding a constant U_0 to a given function $U(\mathbf{r})$, the resulting force and therefore also the work integral W_{12} do not change, because U only appears as a derivative. The scalar function U has the same dimension as the previously defined kinetic energy, hence, it seems reasonable to refer to this quantity as potential energy or simply potential.

To see better when a force field can be written as the gradient of a potential $U(\mathbf{r})$, we consider two paths Γ_A and Γ_B from point 1 to 2. By definition, the work integral W_{12} for a conservative field will be the same for both paths:

$$1 \overbrace{\Gamma_{\mathbf{A}}}^{2} \qquad \int_{\Gamma_{A,1\to 2}} \mathbf{F} \cdot d\mathbf{s} = \int_{\Gamma_{B,1\to 2}} \mathbf{F} \cdot d\mathbf{s}$$
 (91)

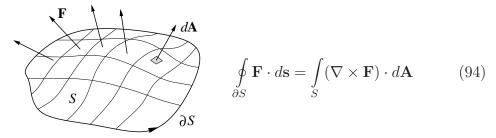
Reversing one of the two paths changes the sign of the work integral:

$$W_{21} = \int_{\Gamma_{-B,2\to 1}} \mathbf{F} \cdot d\mathbf{s} = -\int_{\Gamma_{B,1\to 2}} \mathbf{F} \cdot d\mathbf{s} = -W_{12}$$
(92)

The concatenated path $1 \xrightarrow{\Gamma_A} 2 \xrightarrow{\Gamma_{-B}} 1$ is a closed, and the path integral vanishes:

$$1 \overbrace{\Gamma_{\mathbf{A}}}^{2} \oint_{\Gamma_{-\mathbf{B}}} \mathbf{F} \cdot d\mathbf{s} = W_{12} + W_{21} = 0$$
 (93)

The circle over the integral symbol is a convention indicating the closed path integration. One of the results of vector calculus, referred to as Stokes' theorem, relates the path integral of a vector field \mathbf{F} along the boundary ∂S of an orientable surface S with a surface integral of the curl $\nabla \times \mathbf{F}$ of the field:



As closed path integrals of the type (93) vanish for conservative fields for all paths, the integral over $\nabla \times \mathbf{F}$ on the right side is also identical to zero. This must hold for all surfaces, also sufficiently small ones where $\nabla \times \mathbf{F}$ is smooth, which implies that

$$\nabla \times \mathbf{F} = 0 \tag{95}$$

everywhere. This is an important result: the curl of a conservative force field vanishes – and the other way round, because the Stokes theorem has no logical direction. So all force fields $\mathbf{F}(\mathbf{r})$ with $\nabla \times \mathbf{F} = 0$ are conservative.

One can show easily (by explicitly carrying out the differentiation) that force fields that can be written as the gradient of any potential $U(\mathbf{r})$ are curl-free and thus conservative:

$$\nabla \times [\nabla U(\mathbf{r})] \equiv 0 \tag{96}$$

This justifies the ansatz in (89) to write conservative field as the gradient of a potential. Further, one can show that *every* sufficiently smooth field \mathbf{F} with $\nabla \times \mathbf{F} = 0$ can be represented by a gradient of the form (89).

3.3 Total energy

For conservative fields, we can write the work W_{12} for moving from point 1 to 2 as a difference between the kinetic energy T at the two points due to (85), and as a difference of the potential energy at the two endpoints according to (88):

$$W_{12} = T(\mathbf{r}_2) - T(\mathbf{r}_1) = U(\mathbf{r}_1) - U(\mathbf{r}_2)$$

$$\tag{97}$$

So the change in kinetic energy corresponds to the negative change in the potential energy. Thus, it is reasonable to define a $total\ energy\ E$:

$$E := T + U \tag{98}$$

From (97) it follows immediately that for a transition from point 1 to point 2, the total energy does not change in a conservative force field:

$$E(\mathbf{r}_1) = T(\mathbf{r}_1) + U(\mathbf{r}_1) = T(\mathbf{r}_2) + U(\mathbf{r}_2) = E(\mathbf{r}_2)$$
(99)

Using this equality, it is easy to see that the total energy is the same for every point along a path Γ , and that the temporal derivative dE/dt therefore vanishes — or that the total energy E is conserved.

This derivation assumed that the force is not explicitly time dependent. The statement of conservation of the total energy can be slightly extended to time-dependent potentials. To see that, we first use (82) and transit from differentials to temporal derivatives:

$$dT = \mathbf{F} \cdot d\mathbf{s} \Rightarrow \frac{dT}{dt} = \mathbf{F} \cdot \frac{d\mathbf{r}}{dt} = \mathbf{F} \cdot \dot{\mathbf{r}} = \mathbf{F} \cdot \mathbf{v}$$
 (100)

The total temporal derivative of the potential experienced by a particle moving along a path is composed by both the spatial dependency of U, and its explicit time dependency:

$$\frac{dU}{dt} = \sum_{i} \frac{\partial U}{\partial x_{i}} \frac{dx_{i}}{dt} + \frac{\partial U}{\partial t}$$

$$= (\nabla U) \cdot \mathbf{v} + \frac{\partial U}{\partial t} = -\mathbf{F} \cdot \mathbf{v} + \frac{\partial U}{\partial t}$$
(101)

Adding the last two equations then yields the change of the total energy over time:

$$\frac{dE}{dt} = \frac{dT}{dt} + \frac{dU}{dt} = \frac{\partial U}{\partial t} \tag{102}$$

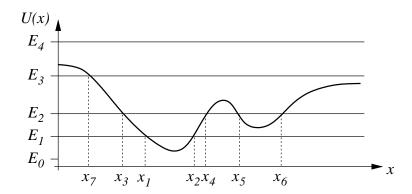
Again, if the potential U does not explicitly depend on time, dE/dt = 0, and the total energy is conserved.

3.3.1 Classification of problems

The knowledge of the potential and the total energy of a system allows making a lot of qualitative statements about the motion of a particle, even without solving the full equation of motion. For this, we consider the potential U(x) in a one-dimensional problem:

First, the system can not have a total energy smaller than the lowest potential U(x) anywhere, because the kinetic energy $T = mv^2/2$ has to be positive. Thus, a system with total energy E_0 has no solution.

For $E = E_1$, there is a region between x_1 and x_2 where $T \ge 0$. The two positions $x_{1,2}$ are called *classical turning points*, because the kinetic energy vanishes there, while the force does not. In such a scenario, the physical system will oscillate between the classical turning points. The solution of the equation of motion



is referred to as a bound solution, because the motion is restricted to the finite interval $[x_1, x_2]$.

For a total energy $E = E_2$, there are two such intervals, $[x_3, x_4]$ and $[x_5, x_6]$. The solution of the equation of motion will have two branches, but there will be no transition between them. Any position x of the system outside these two intervals is not allowed, and said to be forbidden by energy conservation.

For $E = E_3$ (and assuming $U < E_3$ for $x > x_6$), the system has still a classical turning point x_7 , but is not bounded anymore. For $t \to \pm \infty$, the system will evolve to $x \to +\infty$.

For the last case (assuming $U < E_4$ everywhere), there is no restriction to the position x of the system: a particle will come from $x \to -\infty$ and evolve to $x \to +\infty$, or the other way around. The last two cases are often found in scattering problems, since the asymptotic position for $t \to \pm \infty$ is not finite, whereas the interesting part of $U(\mathbf{x})$ is often limited to a small region.

3.3.2 Transit time

The expression of a total energy in a conservative system can be used to evaluate the time it takes a system to evolve between two points, without having to solve the equation of motion explicitly. For a one-dimensional problem and a given potential U(x) and total energy E, one can invert the expression for the total energy,

$$E = \frac{1}{2}mv^2 + U(x) \tag{103}$$

and obtain an expression for the velocity v at a given position:

$$v = \pm \sqrt{\frac{2}{m}(E - U(x))} = \frac{dx}{dt}$$
 (104)

A single integration leads to an expression for the time difference between two positions x, x_0 :

$$t - t_0 = \int_{t_0}^t dt' = \int_{x_0}^x \frac{1}{v} dx' = \int_{x_0}^x \frac{dx'}{\sqrt{\frac{2}{m}(E - U(x))}}$$
 (105)

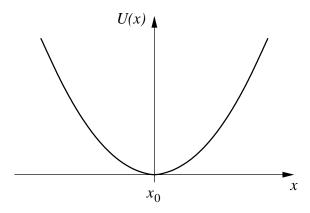
as long as the sign of the velocity does not change over the region $[x_0, x]$. Such an expression can be used to evaluate the oscillation period in an arbitrary potential leading to bound solutions.

3.3.3 Potential of a harmonic oscillator

A particularly important potential U(x) in physics is that of a harmonic oscillator which is characterized by a restoring force $\mathbf{F}(\mathbf{x})$ proportional to its displacement from a reference position $\mathbf{x} = \mathbf{x}_0$. It can easily be seen that the potential

$$U(\mathbf{x}) = \frac{1}{2}k(\mathbf{x} - \mathbf{x}_0)^2 \tag{106}$$

leads to the restoring force $\mathbf{F} = -k (\mathbf{x} - \mathbf{x}_0)$ seen in 2.3.3 for the one-dimensional case.



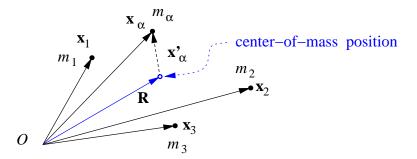
As many local minima (with a non-vanishing second derivative d^2U/dx^2) can be approximated by a parabola, many potentials with a local minimum lead to an approximate harmonic oscillation around this minimum position \mathbf{x}_0 .

4 System of many particles

So far, the mathematical formalism to describe the dynamics of a system was restricted to a single particle. Many times, however, one is interested in the dynamics of a system of many interacting particles. These N particles shall have individual masses m_{α} and individual instantaneous positions \mathbf{x}_{α} , where α is a particle index.

Often, one is not interested in the properties like position or velocity of the individual particles, but in joint properties of the whole ensemble. It is therefore useful to define a few such quantities. Obviously, the $total\ mass\ M$ of the ensemble is given by

$$M := \sum_{\alpha=1}^{N} m_{\alpha} \tag{107}$$



With this, one can define a position vector **R** pointing to the center of mass

$$\mathbf{R} := \frac{1}{M} \sum_{\alpha=1}^{N} m_{\alpha} \mathbf{x}_{\alpha} \tag{108}$$

of the ensemble, which is an average position of all particles, weighted by their mass. One can re-express the individual particle positions \mathbf{x}'_{α} relative to the center of mass:

$$\mathbf{x}_{\alpha} = \mathbf{R} + \mathbf{x}_{\alpha}' \tag{109}$$

4.1 Center-of-mass motion

To obtain the Newtonian equations of motion for the ensemble, one needs to know the force \mathbf{F}_{α} acting each particle α . It is convenient to split this force into a component \mathbf{f}_{α} caused by the interaction between the particles in the ensemble, and a component $\mathbf{F}_{\alpha}^{ext}$ due to external interactions:

$$\mathbf{F}_{\alpha} = \mathbf{F}_{\alpha}^{ext} + \mathbf{f}_{\alpha} \quad \text{with} \quad \mathbf{f}_{\alpha} = \sum_{\substack{\beta \ \beta \neq \alpha}} \mathbf{f}_{\alpha\beta}$$
 (110)

The latter sum considers interactions between particle α with all other particles β . For central forces, like gravitational attraction or Coulomb interaction, these internal forces are symmetric according to Newton's third law:

$$\mathbf{f}_{\alpha\beta} = -\mathbf{f}_{\beta\alpha} \tag{111}$$

The equation of motion for the whole ensemble is then simply the set of equations of motion for the individual particles for all α :

$$m\ddot{\mathbf{x}}_{\alpha} = \mathbf{F}_{\alpha}^{ext} + \sum_{\beta \neq \alpha} \mathbf{f}_{\alpha\beta} \quad \alpha = 1...N$$
 (112)

The summation over all equations in (112) leads on the left side to

$$\sum_{\alpha} m\ddot{\mathbf{x}}_{\alpha} = \frac{d^2}{dt^2} \sum_{\alpha} m\mathbf{x}_{\alpha} = M\ddot{\mathbf{R}}.$$
 (113)

On the right side, we can define a total external force

$$\mathbf{F}^{ext} := \sum_{\alpha} \mathbf{F}_{\alpha}^{ext} \tag{114}$$

The sum over all internal forces $\mathbf{f}_{\alpha\beta}$ vanishes,

$$\sum_{\substack{\alpha,\beta\\\alpha\neq\beta}} \mathbf{f}_{\alpha\beta} = 0, \tag{115}$$

because in the double summation over α and β , each term $\mathbf{f}_{\alpha\beta}$ gets canceled out by the term $\mathbf{f}_{\beta\alpha}$. Thus, the sum over all equations of motion (112) leads to an equation of motion for the center of mass \mathbf{R} of the ensemble where all internal forces between the particles vanish:

$$M\ddot{\mathbf{R}} = \mathbf{F}^{ext} \tag{116}$$

This equation of motion has the same form as the one for a single particle. Similarly to the definition of a momentum for an individual particle, one can define a *total linear momentum*

$$\mathbf{P} := \sum_{\alpha} m_{\alpha} \dot{\mathbf{x}}_{\alpha} = M \dot{\mathbf{R}} \,, \tag{117}$$

with a time derivative that is only determined by the external force:

$$\dot{\mathbf{P}} = M\ddot{\mathbf{R}} = \mathbf{F}^{ext} \tag{118}$$

This allows considering the motion of a whole ensemble (or more precisely, collective properties of the ensemble like \mathbf{R} and \mathbf{P}) in the same way as a single point with mass M.

4.2 Total angular momentum

The individual particles in the ensemble all have a well-defined angular momentum with respect to a coordinate origin O as defined in (73),

$$\mathbf{l}_{\alpha} = \mathbf{x}_{\alpha} \times \mathbf{p}_{\alpha} = \mathbf{x}_{\alpha} \times m_{\alpha} \dot{\mathbf{x}}_{\alpha} \tag{119}$$

The total angular momentum of the ensemble is then given by

$$\mathbf{L} := \sum_{\alpha} \mathbf{l}_{\alpha} \tag{120}$$

This definition can be expressed in terms of the center-of-mass position \mathbf{R} of the ensemble, and the individual displacements \mathbf{x}'_{α} (109):

$$\mathbf{L} = \sum_{\alpha} (\mathbf{R} + \mathbf{x}'_{\alpha}) \times m_{\alpha} (\dot{\mathbf{R}} + \dot{\mathbf{x}}'_{\alpha})$$

$$= \sum_{\alpha} m_{\alpha} \left[\mathbf{R} \times \dot{\mathbf{R}} + \mathbf{x}'_{\alpha} \times \dot{\mathbf{x}}'_{\alpha} \right]$$

$$+ \mathbf{R} \times \left(\sum_{\alpha} m_{\alpha} \dot{\mathbf{x}}'_{\alpha} \right) + \left(\sum_{\alpha} m_{\alpha} \mathbf{x}'_{\alpha} \right) \times \dot{\mathbf{R}}$$
(121)

The expressions in the parentheses are center of mass position of an ensemble with respect to the center of mass position, and

$$\sum_{\alpha} m_{\alpha} \mathbf{x}'_{\alpha} = \sum_{\alpha} m_{\alpha} (\mathbf{x}_{\alpha} - \mathbf{R}) = \sum_{\alpha} m_{\alpha} \mathbf{x}_{\alpha} - \sum_{\alpha} m_{\alpha} \mathbf{R} = M\mathbf{R} - M\mathbf{R} = 0, \quad (122)$$

so the last two terms in (121) vanish. With $P = M\dot{R}$, this leads to

$$\mathbf{L} = \mathbf{R} \times \mathbf{P} + \sum_{\alpha} \mathbf{x}'_{\alpha} \times \mathbf{p}'_{\alpha} \quad (\text{with } \mathbf{p}'_{\alpha} := m_{\alpha} \dot{\mathbf{x}}'_{\alpha}).$$
 (123)

The total angular momentum is therefore the sum of a contribution from the center of mass, and a contribution of the total angular momentum with respect to the center of mass of the ensemble. This will be become important in the Huygens-Steiner theorem for moments of inertia.

To understand the dynamics of the total angular momentum in a differential equation for \mathbf{L} similar to (77), we first consider the temporal derivative of the individual angular momenta:

$$\dot{\mathbf{l}}_{\alpha} = \frac{d}{dt}(\mathbf{x}_{\alpha} \times \mathbf{p}_{\alpha}) = \underbrace{\dot{\mathbf{x}}_{\alpha} \times \mathbf{p}_{\alpha}}_{=0} + \mathbf{x}_{\alpha} \times \dot{\mathbf{p}}_{\alpha}$$
(124)

The first term vanishes because $\mathbf{p}_{\alpha} = m_{\alpha}\dot{\mathbf{x}}_{\alpha}$, and cross products of parallel vectors are zero. By using $\dot{\mathbf{p}}_{\alpha} = \mathbf{F}_{\alpha}$ and the decomposition (110) one obtains

$$\dot{\mathbf{l}}_{\alpha} = \mathbf{x}_{\alpha} \times \left(\mathbf{F}_{\alpha}^{ext} + \sum_{\beta \atop \alpha \neq \beta} \mathbf{f}_{\alpha\beta} \right) \tag{125}$$

and for the derivative of the total angular momentum

$$\dot{\mathbf{L}} = \sum_{\alpha} \dot{\mathbf{I}}_{\alpha} = \sum_{\alpha} \left(\mathbf{x}_{\alpha} \times \mathbf{F}_{\alpha}^{ext} \right) + \sum_{\alpha, \beta \atop \alpha \neq \beta} \mathbf{x}_{\alpha} \times \mathbf{f}_{\alpha\beta} . \tag{126}$$

To see that the last term vanishes, we reorder the summation

$$\sum_{\substack{\alpha,\beta\\\alpha\neq\beta}} A_{\alpha\beta} = \sum_{\substack{\alpha,\beta\\\alpha<\beta}\\\alpha<\beta} A_{\alpha\beta} + \sum_{\substack{\alpha,\beta\\\alpha>\beta}\\\alpha>\beta} A_{\alpha\beta} = \sum_{\substack{\alpha,\beta\\\alpha<\beta}} (A_{\alpha\beta} + A_{\beta\alpha}) . \tag{127}$$

With $A_{\alpha\beta} = \mathbf{x}_{\alpha} \times \mathbf{f}_{\alpha\beta}$ and using the symmetry $\mathbf{f}_{\alpha\beta} = -\mathbf{f}_{\beta\alpha}$ of the inter-particle forces (111), one finds

$$\sum_{\substack{\alpha,\beta\\\alpha\neq\beta}} \mathbf{x}_{\alpha} \times \mathbf{f}_{\alpha\beta} = \sum_{\substack{\alpha,\beta\\\alpha<\beta}} (\mathbf{x}_{\alpha} - \mathbf{x}_{\beta}) \times \mathbf{f}_{\alpha\beta}.$$
 (128)

For central inter-particle forces, $\mathbf{f}_{\alpha\beta}$ is parallel to the distance vector $\mathbf{x}_{\alpha} - \mathbf{x}_{\beta}$ between them, so the cross product vanishes; therefore, the whole sum (128)

vanishes. With the torque $\mathbf{N}_{\alpha}^{ext} := \mathbf{x}_{\alpha} \times \mathbf{F}_{\alpha}^{ext}$ on particle α according to definition (76) caused by the external force $\mathbf{F}_{\alpha}^{ext}$, the change of the total angular momentum with time is given by

$$\dot{\mathbf{L}} = \sum_{\alpha} \mathbf{N}_{\alpha}^{ext} =: \mathbf{N}^{ext} \,. \tag{129}$$

Analog to the single particle case in (77), the total angular momentum of the ensemble with respect to an origin O remains constant if the *total external torque* \mathbf{N}^{ext} with respect to O vanishes.

4.3 Work and total kinetic energy

Similar to the single particle case, we consider the sum of the work for a transition of the ensemble between two configurations a and b:

$$W_{ab} = \sum_{\alpha} \int_{a}^{b} \mathbf{F}_{\alpha} \cdot d\mathbf{x}_{\alpha} \tag{130}$$

Here, the configurations a and b represent sets of positions $\{\mathbf{x}_1, \mathbf{x}_2, \ldots\}$ for all particles evolving in time. The integral is a path integral for the trajectory of particle α in this transition. In exactly the same way as for the single particle case in section 3.1, one replaces the kernel in the integral via

$$\mathbf{F}_{\alpha} \cdot d\mathbf{x}_{\alpha} = dT_{\alpha} \quad \text{with} \quad T_{\alpha} := \frac{1}{2} m_{\alpha} \mathbf{v}_{\alpha}^{2},$$
 (131)

and can express the total work as

$$W_{ab} = \sum_{\alpha} \int_{a}^{b} dT_{\alpha} = T_b - T_a \,, \tag{132}$$

with a $total\ kinetic\ energy\ T$ of a configuration a or b given by the sum of the individual kinetic energies,

$$T := \sum_{\alpha} T_{\alpha} = \sum_{\alpha} \frac{1}{2} m_{\alpha} \mathbf{v}_{\alpha}^{2}. \tag{133}$$

By splitting the velocity of the individual particles into a center-of-mass velocity $\dot{\mathbf{R}}$, and a relative velocity \mathbf{x}'_{α} with respect to the center-of-mass,

$$\mathbf{v}_{\alpha}^{2} = \dot{\mathbf{x}}_{\alpha}^{2} = (\dot{\mathbf{x}}_{\alpha}^{\prime} + \dot{\mathbf{R}}) \cdot (\dot{\mathbf{x}}_{\alpha}^{\prime} + \dot{\mathbf{R}}) = \mathbf{v}_{\alpha}^{\prime 2} + 2\dot{\mathbf{x}}_{\alpha} \cdot \dot{\mathbf{R}} + \dot{\mathbf{R}} \cdot \dot{\mathbf{R}}, \qquad (134)$$

the total kinetic energy becomes

$$T = \sum_{\alpha} \frac{1}{2} m_{\alpha} v_{\alpha}^{\prime 2} + \sum_{\alpha} \frac{1}{2} m_{\alpha} \dot{\mathbf{R}}^{2} + \dot{\mathbf{R}} \frac{d}{dt} \underbrace{\sum_{\alpha} m_{\alpha} \mathbf{x}_{\alpha}^{\prime}}_{=0}$$
$$= \sum_{\alpha} \frac{1}{2} m_{\alpha} v_{\alpha}^{\prime 2} + \frac{1}{2} M \dot{\mathbf{R}}^{2}. \tag{135}$$

So the total kinetic energy is a sum of the kinetic energy of the relative motion of the particles with respect to each other, and the kinetic energy of the center-of-mass motion in the form of a single particle with the total mass M of the ensemble.

4.4 Total potential energy

Analog to the evaluation of the work integral in section 3.2 for a single particle in a conservative force field through a potential, several potentials can be used to describe conservative forces in a particle ensemble. First, the forces on particle α in (130) get split up in external and internal contributions according to (110):

$$W_{ab} = \sum_{\alpha} \int_{a}^{b} \mathbf{F}_{\alpha}^{ext} \cdot d\mathbf{x}_{\alpha} + \sum_{\substack{\alpha,\beta\\\alpha\neq\beta}} \int_{a}^{b} \mathbf{f}_{\alpha\beta} \cdot d\mathbf{x}_{\alpha}$$
 (136)

Conservative external and internal forces can be written as

$$\mathbf{F}_{\alpha}^{ext} = -\nabla_{\alpha} U_{\alpha} \,, \quad \mathbf{f}_{\alpha\beta} = -\nabla_{\alpha} \overline{U}_{\alpha\beta} \,, \tag{137}$$

where ∇_{α} denotes a differentiation with respect to the coordinates \mathbf{x}_{α} of particle α . The two potentials are different functions, where U_{α} represents external potentials, while the $\overline{U}_{\alpha\beta}$ describes the interaction between particles α and β within the ensemble.

The first term in (136) is completely analog to the single particle case:

$$\sum_{\alpha} \int_{a}^{b} \mathbf{F}_{\alpha}^{ext} \cdot d\mathbf{x}_{\alpha} = -\sum_{\alpha} \int_{a}^{b} (\nabla_{\alpha} U_{\alpha}) \cdot d\mathbf{x}_{\alpha} = -\left(\sum_{\alpha} U_{\alpha}\right) \Big|_{a}^{b}$$
(138)

For the second term in (136), the sum gets split up over half of the combinations α, β like in (128),

$$\sum_{\substack{\alpha,\beta\\\alpha\neq\beta}} \mathbf{f}_{\alpha\beta} \cdot d\mathbf{x}_{\alpha} = \sum_{\substack{\alpha,\beta\\\alpha<\beta}} (\mathbf{f}_{\alpha\beta} \cdot d\mathbf{x}_{\alpha} + \mathbf{f}_{\beta\alpha} \cdot d\mathbf{x}_{\beta}) = \sum_{\substack{\alpha,\beta\\\alpha<\beta}} \mathbf{f}_{\alpha\beta} \cdot d(\mathbf{x}_{\alpha} - \mathbf{x}_{\beta}).$$
 (139)

Formally, the total differential $d\overline{U}_{\alpha\beta}$ can be written as

$$d\overline{U}_{\alpha\beta} = \sum_{i} \frac{\partial \overline{U}_{\alpha\beta}}{\partial x_{\alpha,i}} dx_{\alpha,i} + \frac{\partial \overline{U}_{\alpha\beta}}{\partial x_{\beta,i}} dx_{\beta,i}$$
$$= (\nabla_{\alpha} \overline{U}_{\alpha\beta}) \cdot d\mathbf{x}_{\alpha} + (\nabla_{\beta} \overline{U}_{\alpha\beta}) \cdot d\mathbf{x}_{\beta}. \tag{140}$$

For inter-particle central forces, the potential $\overline{U}_{\alpha\beta}$ only depends on the modulus of the distance, $|\mathbf{x}_{\alpha} - \mathbf{x}_{\beta}|$, therefore, $\overline{U}_{\alpha\beta} = \overline{U}_{\beta\alpha}$. Then,

$$\nabla_{\beta} \overline{U}_{\alpha\beta} = \nabla_{\beta} \overline{U}_{\beta\alpha} = -\mathbf{f}_{\beta\alpha} = \mathbf{f}_{\alpha\beta} , \qquad (141)$$

and the total differential $d\overline{U}_{\alpha\beta}$ in (140) becomes

$$d\overline{U}_{\alpha\beta} = -\mathbf{f}_{\alpha\beta} \cdot d\mathbf{x}_{\alpha} + \mathbf{f}_{\alpha\beta} \cdot d\mathbf{x}_{\beta} = -\mathbf{f}_{\alpha\beta} \cdot d(\mathbf{x}_{\alpha} - \mathbf{x}_{\beta})$$
(142)

With this, the second term in the total work in (136) can be written as

$$\sum_{\substack{\alpha,\beta\\\alpha\neq\beta}} \int_{a}^{b} \mathbf{f}_{\alpha\beta} \cdot d\mathbf{x}_{\alpha} = -\sum_{\substack{\alpha,\beta\\\alpha<\beta}} \int_{a}^{b} d\overline{U}_{\alpha\beta} = -\sum_{\substack{\alpha,\beta\\\alpha<\beta}} \overline{U}_{\alpha\beta} \bigg|_{a}^{b}, \qquad (143)$$

so the complete expression for the total work (136) is

$$W_{ab} = -\left(\sum_{\alpha} U_{\alpha}\right)\Big|_{a}^{b} - \sum_{\substack{\alpha,\beta\\\alpha<\beta}} \overline{U}_{\alpha\beta}\Big|_{a}^{b} = -\left.U\right|_{a}^{b} = U_{a} - U_{b},$$

$$(144)$$

where the last U in the expression is a total potential energy

$$U := \underbrace{\sum_{\alpha} U_{\alpha} + \sum_{\substack{\alpha, \beta \\ \alpha < \beta}} \overline{U}_{\alpha\beta}}_{\text{internal}} \tag{145}$$

for a given system state defined by positions $\{x_1, x_2, \ldots\}$ of all particles.

4.5 Energy conservation

As before in case of a single particle, the work in a configuration change can be written both as a difference in total kinetic and total potential energy. Combining (132) and (144) gives

$$W_{ab} = T_b - T_a = U_a - U_b \,, \tag{146}$$

or after reordering

$$T_a + U_a = T_b + U_b \,, \tag{147}$$

which means the total energy E := T + U of the many-particle system is conserved in an evolution between states a and b.

It should be noted that for *rigid bodies*, the second term in (136) will vanish because the inter-particle distances $||\mathbf{x}_{\alpha} - \mathbf{x}_{\beta}||$ will not change in a system state change $a \to b$. Thus, the contribution (145) due to the internal interactions stay constant, and need not to be evaluated explicitly. Then, the total kinetic and total potential energy in the system are just the sum of the individual contributions from the participating particles.

5 Lagrangian mechanics - first approach

So far, the equations of motion have been derived from Newton's laws, and required the knowledge of forces for all particles. This can sometimes become challenging, in particular in cases where forces need to be considered that are only there to meet the constraints. In general, the equations of motion of a system following Newtonian mechanics can be written as

$$m_k \, \ddot{x_k} = F_k(\{x_l, \dot{x_l}\}, t) \,.$$
 (148)

This is a system of differential equations for all x_k , where k indexes both the coordinate components (like x, y, z) and a particle index in a many particle system: a system of two particles moving in 3-dimensional space would lead to 6 differential equations. The notation $\{x_l, \dot{x}_l\}$ indicates that in principle, all forces F_k can depend on coordinates x_l and velocities \dot{x}_l of all particles. Additionally they can explicitly depend on time t.

Similarly, the total kinetic energy of the system (133) can be written as

$$T = T(\{\dot{x}_l\}) = \sum_k T_k = \sum_k \frac{1}{2} m_k \dot{x}_k^2.$$
 (149)

The Cartesian momentum component for coordinate index k is then given by

$$p_k = m_k \dot{x}_k = \frac{\partial T}{\partial \dot{x}_k} \,, \tag{150}$$

because differentiation of the sum in (149) with respect to \dot{x}_l vanish for $l \neq k$. The left side of (148) can be expressed by the total temporal derivative of (150),

$$m_k \ddot{x}_k = \dot{p}_k = \frac{d}{dt} \left(\frac{\partial T}{\partial \dot{x}_k} \right) = F_k(\{x_l, \dot{x}_l\}, t).$$
 (151)

For conservative forces, one can write $F_k = -\partial U/\partial x_k$, with a total potential energy U for the whole system. This is compatible with the definition in (145). Then, the equations of motion become

$$\frac{d}{dt} \left(\frac{\partial T}{\partial \dot{x_k}} \right) = -\frac{\partial U}{\partial x_k} \quad \text{for all } k.$$
 (152)

With the definition of a so-called Lagrange function L := T - U, this can be written as

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}_k} \right) - \frac{\partial L}{\partial x_k} = 0 \quad \text{for all } k \,, \tag{153}$$

because for the differentiation with respect to $\dot{x_k}$, there is no contribution from U, and similarly, for the differentiation with respect to x_k , there is no contribution

from T. The set (153) is called Lagrange equations of motion of a physical system, and are equivalent to the equation of motion (148) in Newtonian mechanics.

So far, there is no obvious advantage of this method for obtaining the equations of motion. However, it will simplify the treatment of systems, because these equations of motion take the same form in also in general, possibly non-Cartesian coordinates that reflect better the symmetry of a system.

5.1 Example: harmonic oscillator

We consider again the one-dimensional harmonic oscillator. The kinetic energy is given by $T = mv^2/2$, and the potential energy according to (106) by $U = kx^2$ for an equilibrium position $x_0 = 0$. Then, the Lagrange function becomes

$$L = T - U = \frac{1}{2}m\,\dot{x}^2 - \frac{1}{2}k\,x^2 \tag{154}$$

The corresponding Lagrange equation is then

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_k}\right) - \frac{\partial L}{\partial x_k} = \frac{d}{dt}\left(m\,\dot{x}\right) + kx = m\,\ddot{x} + kx = 0\,,\tag{155}$$

which is equivalent to (64).

5.2 Generalization to some non-conservative forces

With the Lagrange formalism, it is also possible to consider some non-conservative velocity-dependent forces, as long as they can be written as

$$F_k = F_k(\{x_l, \dot{x}_l\}, t) = -\frac{\partial V}{\partial x_k} + \frac{d}{dt} \frac{\partial V}{\partial \dot{x}_k}$$
(156)

where $V = V(\{x_l, \dot{x}_l\}, t)$ is a velocity-dependent pseudo-potential. With a Lagrange function L = T - V, the force on the left side of the Newtonian equation of motion (151) can be written as

$$m_k \ddot{x}_k = \frac{d}{dt} \frac{\partial T}{\partial \dot{x}_k} = \frac{d}{dt} \frac{\partial L}{\partial \dot{x}_k} + \frac{d}{dt} \frac{\partial V}{\partial \dot{x}_k}$$
(157)

With the right side of the Newtonian equation of motion (151) taken from (156), and observing that $\partial L/\partial x_k = -\partial V/\partial x_k$ because T does not depend on x_k , one finds

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}_k} + \frac{d}{dt}\frac{\partial V}{\partial \dot{x}_k} = -\frac{\partial V}{\partial x_k} + \frac{d}{dt}\frac{\partial V}{\partial \dot{x}_k} = \frac{\partial L}{\partial x_k} + \frac{d}{dt}\frac{\partial V}{\partial \dot{x}_k}.$$
 (158)

By removing the second derivatives of V on both sides, one ends up with the Lagrange equation of motion of the form (153).

This expands the usefulness of the Lagrange formalism significantly beyond conservative forces. An important example of such a force is the one felt by a charged particle in the presence of both an electrical and magnetic field.

5.2.1 Lagrange function for a charge under electromagnetic forces

A particle with a point charge q is subject to forces both due to electrical and magnetic fields:

$$\mathbf{F} = q\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right) \tag{159}$$

The first part is due to the electric field vector \mathbf{E} , the second part is the Lorentz force due to the presence of a magnetic field \mathbf{B} .

In order to show that such an interaction can be written in a Lagrangian form, we make use from a result from electrodynamics that the electric and magnetic fields can be derived from two potentials,

$$\mathbf{E} = -\nabla \Phi - \frac{\partial}{\partial t} \mathbf{A}, \quad \text{and} \quad \mathbf{B} = \nabla \times \mathbf{A},$$
 (160)

where $\Phi = \Phi(\mathbf{x}, t)$ is the scalar electrical potential, and $\mathbf{A} = \mathbf{A}(\mathbf{x}, t)$ the so-called vector potential. We will show that a "pseudopotential" energy

$$V = V(\mathbf{x}, \dot{\mathbf{x}}, t) = q \left[\Phi(\mathbf{x}, t) - \dot{\mathbf{x}} \cdot \mathbf{A}(\mathbf{x}, t) \right]$$
(161)

can reproduce the electromagnetic force (159) via (156). For this, we first rewrite (159) in terms of individual components k, and express the fields \mathbf{E}, \mathbf{B} by the potentials Φ, \mathbf{A} according to (160):

$$F_{k} = q \left[E_{k} + \sum_{l,m} \epsilon_{klm} \dot{x}_{l} B_{m} \right]$$

$$= q \left[\left(-\frac{\partial \Phi}{\partial x_{k}} - \frac{\partial A_{k}}{\partial t} \right) + \sum_{l,m} \epsilon_{klm} \dot{x}_{l} \left(\sum_{p,q} \epsilon_{mpq} \frac{\partial A_{q}}{\partial x_{p}} \right) \right]$$

$$= q \left[\left(-\frac{\partial \Phi}{\partial x_{k}} - \frac{\partial A_{k}}{\partial t} \right) + \sum_{l,p,q} \left(\sum_{m} \epsilon_{klm} \epsilon_{mpq} \right) \dot{x}_{l} \frac{\partial A_{q}}{\partial x_{p}} \right]$$
(162)

By using an identity for the sum over the Levi-Civita symbols,

$$\sum_{m} \epsilon_{klm} \epsilon_{mpq} = \sum_{m} \epsilon_{mkl} \epsilon_{mpq} = \delta_{kp} \delta_{lq} - \delta_{kq} \delta_{lp}, \qquad (163)$$

the summations over p and q can be removed:

$$F_k = q \left[\left(-\frac{\partial \Phi}{\partial x_k} - \frac{\partial A_k}{\partial t} \right) + \sum_l \dot{x}_l \left(\frac{\partial A_l}{\partial x_k} - \frac{\partial A_k}{\partial x_l} \right) \right]$$
(164)

In a next step, we derive the force via (156) from the pseudopotential V in (161):

$$F_{k} = -\frac{\partial V}{\partial x_{k}} + \frac{d}{dt} \frac{\partial V}{\partial \dot{x}_{k}}$$

$$= q \left[-\frac{\partial \Phi}{\partial x_{k}} + \sum_{l} \dot{x}_{l} \frac{\partial A_{l}}{\partial x_{k}} - \frac{d}{dt} A_{k} \right]$$

$$= q \left[-\frac{\partial \Phi}{\partial x_{k}} + \sum_{l} \dot{x}_{l} \frac{\partial A_{l}}{\partial x_{k}} - \frac{\partial A_{k}}{\partial t} - \sum_{l} \frac{\partial A_{k}}{\partial x_{l}} \dot{x}_{l} \right], \qquad (165)$$

which is exactly the same as the force derived from the fields in (164). Therefore, the forces (159) can be expressed via the pseudopotential (161).

As a consequence, the Lagrange function or *Lagrangian* for a charged particle in time-dependent electromagnetic fields is given by

$$L = T - V = \frac{1}{2}m\dot{\mathbf{x}}^2 - q\left[\Phi(\mathbf{x}, t) - \dot{\mathbf{x}} \cdot \mathbf{A}(\mathbf{x}, t)\right], \qquad (166)$$

and an equation of motion for it can be obtained via the Lagrange equations.

6 Lagrangian mechanics from Hamilton's principle

In the previous section, the dynamics of a physical system was expressed not via equations of motion provided by Newton's laws, but via the definition of a the Lagrange function $L = L(\{x_l, \dot{x}_l\}, t) = T - U$, and a set of differential equations, the so-called Lagrange equations (153).

Since the Lagrange equations are just a mathematical prescription how to obtain equations of motion for a system, all the information on how a system evolves is encoded in the form of the Lagrange function. So far, we used Newton's laws, which use forces as their central concept, to derive the Lagrange equations. However, the forces do not appear in the final equation of motion. Thus, several attempts were made to derive the equations of motion from different principles, and that do not require the notion of forces.

A long-time popular concept is the principle of minimizing a certain quantity: For example, to explain how light is reflected off a mirror, Hero³ postulated that the light takes the shortest path between two points. About 1000 years later, this principle was extended by Ibn al-Haytham⁴ to describe the refraction of light as well, postulating the principle that the path of the light is determined by the shortest time to move between two points. This was stated in a modern from by Fermat⁵ and is known as *Fermat's principle*.

After a number of attempts to come up with such a principle determining the mechanics by physicists over the time, Hamilton⁶ announced in 1834/35 the dynamic principle, often referred to as Hamilton's principle, that does exactly this. It basically states:

Of all possible paths a system may move from one point to another within a specified time interval, the actual path followed is the one that minimizes the integral over the difference between kinetic and potential energies.

³Hero of Alexandria, ≈ 10 -70, in year 60

⁴Ibn al-Haytham from Cairo, 965-1040

⁵Pierre de Fermat, Toulouse, France, 1601-1665

⁶Sir William Rowan Hamilton, 1805-1865

A mathematical formulation of this is often written as

$$\delta S = 0$$
, with $S := \int_{t_1}^{t_2} (T - U) dt = \int_{t_1}^{t_2} L dt$, (167)

where the time integral S is referred to as action of a physical system when evolving between two different states at times t_1 and t_2 . The delta symbol here refers somewhat vaguely to a variation of a quantity, which tries to capture what is meant by "the trajectory chosen by nature of the system will make S extremal". The quantity δS is the change of S with a variation of the final trajectory, and should vanish for the extremal path – in a similar way that the change df of a function f(x) vanishes with variation $x \to x + dx$ near a minimum or maximum of f(x). The mathematical discipline of $variational\ calculus$ tries to solve exactly this problem.

6.1 Elements of variational calculus - Euler equation

To solve the variational problem of a kind proposed by Hamilton's principle, we first consider a function y(x), and a recipe to obtain a number J from this function,

$$J = \int_{x_1}^{x_2} f(y(x), y'(x), x) dx, \qquad (168)$$

where f is a function that depends on three parameters: the function y(x) itself, its derivative y'(x) with respect to the function parameter x, and x itself. Such a function is referred to as a functional. Examples for such functions would be

$$f = y\sqrt{(1+y'^2)}$$
 or $f = \sqrt{\frac{1+y'^2}{x}}$, (169)

where the first one does not explicitly depend on x, and the second one not explicitly on y.

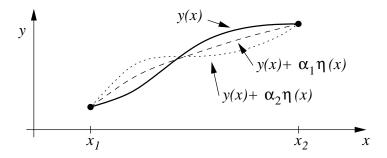
To find a condition on y(x) that minimizes or maximizes the value J, we consider a small deviation of y(x) from that optimum in the form of a variation

$$y(\alpha, x) = y(x) + \alpha \eta(x), \qquad (170)$$

where α is a parameter to gradually add the "deviation" $\eta(x)$ to the optimal solution y(x). At the end points $x_{1,2}$, the deviation should vanish, $\eta(x_1) = \eta(x_2) = 0$.

Now, the functional J becomes a function of the perturbation parameter α ,

$$J(\alpha) = \int_{x_1}^{x_2} f(y(\alpha, x), y'(\alpha, x), x) dx, \qquad (171)$$



For a function y(x) that makes J extremal, one would require the condition

$$\frac{\partial J}{\partial \alpha}\Big|_{\alpha=0} \stackrel{!}{=} 0 \quad \text{for all} \quad \eta(x) \,, \tag{172}$$

because a small change from the optimal y(x) will not change the value of J at the optimum. Condition (172) will now lead to a way to construct y(x):

$$\frac{\partial J}{\partial \alpha} = \int_{x_1}^{x_2} \left(\frac{\partial f}{\partial y} \frac{\partial y}{\partial \alpha} + \frac{\partial f}{\partial y'} \frac{\partial y'}{\partial \alpha} \right) dx = \int_{x_1}^{x_2} \left(\frac{\partial f}{\partial y} \underbrace{\frac{\partial y}{\partial \alpha}}_{=\eta(x)} + \frac{\partial f}{\partial y'} \underbrace{\frac{\partial^2 y}{\partial \alpha \partial x}}_{=\frac{d\eta(x)}{dx}} \right) dx$$

$$= \int_{x_1}^{x_2} \left(\frac{\partial f}{\partial y} \eta(x) \right) dx + \int_{x_1}^{x_2} \left(\frac{\partial f}{\partial y'} \frac{d\eta(x)}{dx} \right) dx \tag{173}$$

The last part can be integrated using $u = \partial f/\partial y', v = \eta(x)$, and $\int uv' = uv - \int u'v$:

$$\frac{\partial J}{\partial \alpha} = \int_{x_1}^{x_2} \left(\frac{\partial f}{\partial y} \eta(x) \right) dx + \underbrace{\frac{\partial f}{\partial y'} \eta(x)}_{x_1} \Big|_{x_1}^{x_2} - \int_{x_1}^{x_2} \left(\frac{d}{dx} \frac{\partial f}{\partial y'} \right) \eta(x) dx$$

$$= \int_{x_1}^{x_2} \left(\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y'} \right) \eta(x) dx \tag{174}$$

To make J extremal, $\partial J/\partial \alpha$ needs to vanish for all deviations $\eta(x)$, and thus the expression in the parentheses needs to vanish. As the expression has to be evaluated for $\alpha = 0$, the expression in parentheses leads to a differential equation for the *optimal* y(x):

$$\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y'} = 0 \tag{175}$$

This condition is called the *Euler equation*, and provides a differential equation to find the function y(x) that maximizes or minimizes J. This is a purely mathematical result. For $f = L(x, \dot{x}, t)$, (175) has exactly the form of the Lagrange equation (153) derived from Newton's laws earlier. Therefore, in a mechanics context, the equations of motion of this form are also called *Euler-Lagrange equations*.

6.1.1 Second from of the Euler equation

The Euler equation (175) can be simplified if the function f does not explicitly depend on x:

$$f = f(y, y') \tag{176}$$

To arrive there, one starts with the total differential

$$\frac{df}{dx} = \underbrace{\frac{\partial f}{\partial x}}_{=0} + \underbrace{\frac{\partial f}{\partial y}}_{y'} y' + \underbrace{\frac{\partial f}{\partial y'}}_{y'} y''. \tag{177}$$

The first term vanishes because f does not explicitly depend on x. By evaluating

$$\frac{d}{dx}\left(y'\frac{\partial f}{\partial y'}\right) = y''\frac{\partial f}{\partial y'} + y'\frac{d}{dx}\frac{\partial f}{\partial y'}$$
(178)

and substituting the first term on the right side with the last term in (177), one finds

$$\frac{d}{dx}\left(y'\frac{\partial f}{\partial y'}\right) = \frac{df}{dx} - \frac{\partial f}{\partial y}y' + y'\frac{d}{dx}\frac{\partial f}{\partial y'}$$

$$= \frac{df}{dx} + y'\underbrace{\left(\frac{d}{dx}\frac{\partial f}{\partial y'} - \frac{\partial f}{\partial y}\right)}_{0} \tag{179}$$

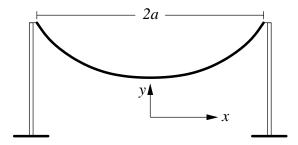
The last term vanishes because of the Euler equation (175). The rest can be written as

$$\frac{d}{dx}\left(f - y'\frac{\partial f}{\partial y'}\right) = 0 \quad \text{or} \quad f - y'\frac{\partial f}{\partial y'} = const. \tag{180}$$

This is the so-called *second from* of the Euler equation for y(x) to minimize/maximize the functional J in (168).

6.1.2 Example: shape of a heavy rope

As a simple example for a variational problem, we consider the shape of a heavy chain or rope suspended between two poles:



The principle that defines the shape of the rope is the demand that the potential energy of the chain at rest should be minimal, because all deviations from that configuration would drive the system into motion, which would eventually be converted into heat via friction. The problem is completely defined by specifying the length l of the rope, and the spacing 2a < l between the poles.

The total potential energy U in the gravitational acceleration g of the rope with a line density (i.e., mass per length) ρ is given by

$$U = \int \rho \, g \, y \, ds \,, \tag{181}$$

where the integration is carried out along the rope, with a line element ds. This integration along the rope can be expressed by an integration along x with the line element $ds = \sqrt{dx^2 + dy^2} = \sqrt{1 + y'^2} dx$:

$$dy \int_{-a}^{a} y \sqrt{1 + y'^2} dx$$
 (182)

This is a variational problem of the "second form" (180) with $f = y\sqrt{1 + y'^2}$. With the constant c required by the Euler equation in the second form, we get

$$c = f - y' \frac{\partial f}{\partial y'} = y\sqrt{1 + y'^2} - y' \frac{yy'}{\sqrt{1 + y'^2}}$$
$$= \frac{y(1 + y'^2)}{\sqrt{1 + y'^2}} - \frac{yy'^2}{\sqrt{1 + y'^2}} = \frac{y}{\sqrt{1 + y'^2}}, \tag{183}$$

which can be further transformed into

$$cy' = c\frac{dy}{dx} = \sqrt{y^2 - c^2}$$
 or $\frac{c\,dy}{\sqrt{y^2 - c^2}} = dx$ (184)

Integration on both sides leads to

$$\operatorname{arccosh} \frac{y}{c} = \frac{1}{c}(x + x_0) \tag{185}$$

or finally

$$y(x) = c \cosh\left(\frac{x+x_0}{c}\right), \tag{186}$$

with the two integration constants c and x_0 . Since $\cosh z = (e^z + e^{-z})/2$ is an even function, we choose $x_0 = 0$ in the middle of the rope. To fix the final constant c from the rope length, we need an expression for the length, and with $y' = \sinh(x/c)$ we find

$$l = \int_{-a}^{a} \sqrt{1 + y'^2} \, dx = \int_{-a}^{a} \sqrt{1 + \sinh^2 \frac{x}{c}} \, dx = \int_{-a}^{a} \cosh \frac{x}{c} \, dx$$
$$= c \sinh \frac{x}{c} \Big|_{-a}^{a} = 2c \sinh \frac{a}{c} \tag{187}$$

This leads to a transcendental equation

$$\sinh z = z \frac{l}{2a} \quad \text{with} \quad z = \frac{a}{c}, \tag{188}$$

which finally has to be solved numerically for z and consequently c.

6.1.3 Euler equations with several dependent variables

The Lagrange equations (153) typically involve several dependent variables, i.e., all coordinates of all particles. This corresponds to N individual functions $y_k(x)$ that all depend on the same x. The functional f in (168),

$$f = f(\{y_k(x), y_k'(x)\}; x) , \qquad (189)$$

depends now on an ensemble $\{y_k(x), y'_k(x)\}$ of variables y_k and their derivatives y'_k with respect to x in the same way as in (148). For the variational argument, one defines a variation for component y_k in the same way as in (170),

$$y_k(\alpha, x) = y_k(x) + \alpha \eta_k(x). \tag{190}$$

The requirement to the extremal condition on J in (168) becomes

$$\frac{\partial J}{\partial \alpha} = \int_{x_k}^{x_2} \sum_{k} \left(\frac{\partial f}{\partial y_k} - \frac{d}{dx} \frac{\partial f}{\partial y_k'} \right) \eta_k(x) \, dx \stackrel{!}{=} 0.$$
 (191)

Since all deviation functions $\eta_k(x)$ are independent, all the parentheses in the sum above have to vanish, which results in a system of differential equations:

$$\frac{\partial f}{\partial y_k} - \frac{d}{dx} \frac{\partial f}{\partial y'_k} = 0 \quad \text{for all} \quad k = 1 \dots N$$
 (192)

This is exactly of the form that allows deriving the Lagrange equations from the Hamilton principle in (167), where f becomes the Lagrange function $L(\{x_k, \dot{x}_k\}, t)$, and the independent variable x is replaced with time t.

6.2 Generalized coordinates

The Hamilton principle states that a physical system takes the trajectory that makes the variation of the action integral vanish:

$$\delta S = \delta \int_{t_1}^{t_2} L \, dt = \delta \int_{t_1}^{t_2} (T - U) \, dt = 0.$$
 (193)

Earlier, the scalar Lagrange function L was expressed in a set of Cartesian coordinates, $\{x_k\}$, and a set of corresponding velocities, $\{\dot{x}_k\}$, and eventually the

time t explicitly. Then, the Euler-Lagrange equations (192) provide equations of motion for the whole physical system:

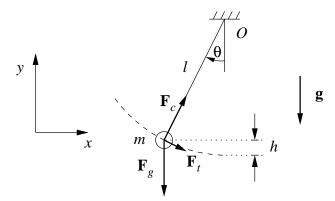
$$\frac{\partial L}{\partial x_k} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}_k} = 0 \quad \text{for all} \quad k = 1 \dots N$$
 (194)

These equations of motion are equivalent to the equations of motion we derived out of Newton's laws, so there would be no advantage in introducing a new principle to derive the equations of motion of a system.

In the variational calculus argument, there was no explicit reference that Cartesian coordinates needed to be used to write down the Lagrange function. The Euler-Lagrange equations (194) were obtained buy simply replacing the y_k in (192) by coordinates x_k , and similarly their derivatives with respect to the independent parameter, and switching to the independent variable t. The Hamilton principle does, however, not state anywhere that the Cartesian coordinates have to be used for describing the system. Therefore, it is fine to use other coordinates to describe the system, and the Hamilton principle provides a way to find the equations of motion in other than Cartesian coordinate systems. This is an important advantage of the Hamilton principle in comparison to the approach by using Newton's laws.

6.2.1 Simple example: plane pendulum

To demonstrate this, we consider the relatively simple problem of a pendulum, made up by a mass m on a massless string of length l in the gravitational acceleration \mathbf{g} :



To come up with the equation of motion from Newton's laws, we first recognize that the motion of the mass is constrained on a circular trajectory. An adequate coordinate to express this is the angle θ , with a fixed distance l to the origin. Forces acting on the particle are the force $\mathbf{F}_g = m\mathbf{g} = -mg\,\mathbf{e}_y$ induced by the gravitational acceleration \mathbf{g} , and a constraining force \mathbf{F}_c exerted by the string on the mass to keep it on a circular trajectory, which is aligned with the string,

$$\mathbf{F}_c = -F_c \,\mathbf{e}_r = -F_c \,(\mathbf{e}_{\mathbf{x}} \sin \theta - \mathbf{e}_{\mathbf{y}} \cos \theta). \tag{195}$$

For a circular motion, r = l = const., and therefore $\dot{r} = 0$ and $\ddot{r} = 0$. According to (28), the projection $a_r = \ddot{\mathbf{x}} \cdot \mathbf{e}_r$ of the total acceleration $\ddot{\mathbf{x}}$ in radial direction is given by $a_r = \ddot{r} - r\dot{\theta}^2 = -l\dot{\theta}^2$. With the constraining force pointing in inverse radial direction, $\mathbf{F}_c = -F_c \mathbf{e}_r$, one can determine its amplitude F_c :

$$(\mathbf{F}_{g} + \mathbf{F}_{c}) \cdot \mathbf{e}_{r} = (m \, \ddot{\mathbf{x}}) \cdot \mathbf{e}_{r}$$

$$-mg (\mathbf{e}_{y} \cdot \mathbf{e}_{r}) - F_{c} = m \, a_{r}$$

$$-mg (-\cos \theta) - F_{c} = -m \, l\dot{\theta}^{2}$$

$$F_{c} = m (g \cos \theta + l\dot{\theta}^{2}). \tag{196}$$

With knowledge of F_c , we can finally evaluate the total force, and use Newton's law to make the connection to the acceleration $\ddot{\mathbf{x}}$, again using (28):

$$m \ddot{\mathbf{x}} = \mathbf{F}_g + \mathbf{F}_c$$

$$m \left(-l\dot{\theta}^2 \mathbf{e}_r + l\ddot{\theta} \mathbf{e}_{\theta} \right) = -mg \mathbf{e}_y - m \left(g \cos \theta + l\dot{\theta}^2 \right) \mathbf{e}_r$$
(197)

The terms with $l\dot{\theta}^2$ cancel, and by multiplying the last equation with $\mathbf{e}_{\theta} = -\mathbf{e}_x \cos \theta + \mathbf{e}_y \sin \theta$, dividing by m and using $\mathbf{e}_r \cdot \mathbf{e}_{\theta} = 0$, we get

$$l\ddot{\theta} = -g\left(\mathbf{e}_{y} \cdot \mathbf{e}_{\theta}\right) = -g\sin\theta\tag{198}$$

or finally

$$\ddot{\theta} + \frac{g}{I}\sin\theta = 0. \tag{199}$$

Steps (195) and (196) may seem unnecessarily complicated, because the constraining force was explicitly calculated, but this would be the procedure according to Newton's laws, taking care of all forces acting on the mass. One could have cut some corners by only looking at the projection of all forces on \mathbf{e}_{θ} , and notice that the only force that contributes here would be \mathbf{F}_{g} , while the constraining force is orthogonal to \mathbf{e}_{θ} , and would not need to be evaluated explicitly.

Now, we compare the strategy to obtain the equation of motion with the one provided by the Lagrange formalism. We start out with writing down the kinetic energy,

$$T = \frac{1}{2}mv^2 = \frac{1}{2}ml^2\dot{\theta}^2\,, (200)$$

and the potential energy of a mass in gravitational acceleration,

$$U = mgh - U_0 = mgl(1 - \cos\theta) - U_0 = -mgl\cos\theta, \qquad (201)$$

where we could subtract the constant offset $U_0 = mgl$ because this does not affect the dynamics of the system. The Lagrange function then can be written as

$$L = T - U = \frac{1}{2}ml^2\dot{\theta}^2 + mgl\cos\theta, \qquad (202)$$

which is now only a function of the dynamic variables θ and $\dot{\theta}$. Since Hamilton's principle makes no statement what coordinates can be used, as long as one can define a meaningful potential and kinetic energy, one could just use (194) for the single variable θ , and get the Euler-Lagrange equations of motion:

$$\frac{\partial L(\theta, \dot{\theta})}{\partial \theta} - \frac{d}{dt} \frac{\partial L(\theta, \dot{\theta})}{\partial \dot{\theta}} = 0.$$
 (203)

By carrying out the differentiations of L, one finds

$$-mgl\sin\theta - \frac{d}{dt}ml^2\dot{\theta} = -mgl\sin\theta - ml^2\ddot{\theta} = 0.$$
 (204)

Dividing the last part by $-ml^2$, we reproduce the equation of motion (199):

$$\ddot{\theta} + \frac{g}{l}\sin\theta = 0. \tag{205}$$

In this derivation, there was no need to work out any forces. A lucky choice of the right coordinate, θ in this case, took implicitly care of the constraint that the mass has to move on a circle.

6.2.2 Generalized coordinates and velocities

The treatment of the pendulum above is only an example of describing a system by generalized coordinates, which are usually referred to as a set $\{q_k\}$. Together with the set of their corresponding temporal derivatives, $\{\dot{q}_k\}$, referred to as generalized velocities, they give a complete description of the state of a physical system at any point in time. Again, the system can be made up by a number of particles. Then, Hamilton's principle leads directly to a set of equations of motion for the whole system:

$$\frac{\partial L}{\partial q_k} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_k} = 0 \quad \text{for all} \quad k = 1 \dots N$$
 (206)

A few remarks on generalized coordinates seem to be in order:

- Generalized coordinates do not need to have the dimension of a length, like Cartesian coordinates do by specifying the respective distance from a reference point to the position of a mass point.
- Likewise, generalized velocities do not need to have the dimension of a length per time, the dimension of the traditional velocity.
- Generalized coordinates of a particle can be functions of various coordinates of one particle, but can also be combinations of coordinates from different particles.

- To some extent, generalized coordinates may explicitly contain the time.
- Generalized coordinates may be used to take care of constraints of a system, like in the pendulum example. A careful analysis of the degrees of freedom of a system can eliminate the explicit need to consider constraints.

The only thing that is really required for generalized coordinates to be useful for coming up with the equations of motion of a physical system is that all the degrees of freedom of the system are properly captured, and that it is possible to formulate a Lagrange function that only depends on the $\{q_k\}$ and $\{\dot{q}_k\}$.

6.2.3 Point transformations between traditional and generalized coordinates

One can make the transition between the traditional Cartesian coordinates $\{x_k\}$ and the generalized coordinates $\{q_k\}$ of a system slightly more explicit by introducing a specific transformation between the two sets, and then showing that the Euler-Lagrange equations in the generalized coordinates follow from the Euler-Lagrange equations in the original coordinates. This step, however, is not necessary to see that (206) can describe the complete dynamics of a system, but it illustrates what transformations can be used to construct generalized coordinates.

A property for a set of generalized coordinates $\{\dot{q}_k\}$ is that all the degrees of freedom of the system are captured. Then, there must exist a transformation that converts between the old and new set of coordinates, so the old coordinates may be expressed as a function of the new coordinates, and possible the time t:

$$x_k = x_k(\{q_l\}, t) (207)$$

This notation means that x_k is an explicit function of all the q_l , and the time t. Then, the temporal derivative of q_k can be calculated:

$$\dot{x}_k = \frac{\partial x_k}{\partial t} + \sum_l \frac{\partial x_k}{\partial q_l} \frac{dq_l}{dt} = \frac{\partial x_k}{\partial t} + \sum_l \frac{\partial x_k}{\partial q_l} \dot{q}_l$$
 (208)

This makes \dot{x}_k an explicit function of the set $\{q_l\}$ (via the derivatives of x_k with respect to q_l), the set $\{\dot{q}_l\}$, and the time. The Lagrange function in the old coordinates, L, and the one in new coordinates, L', should be the same, but of course the functions L and L' take a different form in the respective coordinate sets – this is why there is a different symbol, L':

$$L(\lbrace x_k \rbrace, \lbrace \dot{x}_k \rbrace, t) = L(\lbrace x_k(\lbrace q_l \rbrace, t) \rbrace, \lbrace \dot{x}_k(\lbrace q_l \rbrace, \lbrace \dot{q}_l \rbrace, t) \rbrace) = L'(\lbrace q_l \rbrace, \lbrace \dot{q}_l \rbrace, t)$$
 (209)

We now evaluate the derivatives we need for the Euler-Lagrange equations in the new coordinates:

$$\frac{\partial L'}{\partial q_l} = \sum_{k} \frac{\partial L}{\partial x_k} \frac{\partial x_k}{\partial q_l} + \frac{\partial L}{\partial \dot{x}_k} \frac{\partial \dot{x}_k}{\partial q_l}$$
(210)

and

$$\frac{\partial L'}{\partial \dot{q}_l} = \sum_{k} \left(\frac{\partial L}{\partial x_k} \underbrace{\frac{\partial x_k}{\partial \dot{q}_l}}_{=0} + \frac{\partial L}{\partial \dot{x}_k} \underbrace{\frac{\partial \dot{x}_k}{\partial \dot{q}_l}}_{=\partial x_k/\partial q_l} \right) = \sum_{k} \left(\frac{\partial L}{\partial \dot{x}_k} \frac{\partial x_k}{\partial q_l} \right)$$
(211)

The first term vanishes because in (207), x_k does not explicitly depend on the velocity \dot{q}_l . The change in the second derivative can be seen from (208) because the only term in \dot{x}_k that depends on \dot{q}_l is the one with $\partial x_k/\partial q_l$ (don't get confused with the same l index – in (208), this is a summation index, and can be replaced with, say, m. Then, $\partial \dot{q}_m/\partial q_l = \delta_{lm}$ and the sum vanishes...).

Then, the "new" Euler-Lagrange equation can then simply be calculated:

$$\frac{\partial L'}{\partial q_l} - \frac{d}{dt} \frac{\partial L'}{\partial \dot{q}_l} = \sum_{k} \left(\frac{\partial L}{\partial x_k} \frac{\partial x_k}{\partial q_l} + \frac{\partial L}{\partial \dot{x}_k} \frac{\partial \dot{x}_k}{\partial q_l} \right) - \frac{d}{dt} \left(\sum_{k} \frac{\partial L}{\partial \dot{x}_k} \frac{\partial x_k}{\partial q_l} \right) \\
= \sum_{k} \left[\frac{\partial x_k}{\partial q_l} \left(\underbrace{\frac{\partial L}{\partial x_k} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}_k}}_{=0} \right) + \frac{\partial L}{\partial \dot{x}_k} \left(\frac{\partial \dot{x}_k}{\partial q_l} - \frac{d}{dt} \frac{\partial x_k}{\partial q_l} \right) \right] (212)$$

The first parenthesis vanishes because of the Euler-Lagrange equations in the original coordinates $\{x_k\}$. For the second term, one explicitly calculates

$$\frac{d}{dt}\frac{\partial x_k}{\partial q_l} = \frac{\partial^2 x_k}{\partial q_l \partial t} + \sum_m \frac{\partial^2 x_k}{\partial q_l \partial q_m} \dot{q}_m$$

$$= \frac{\partial}{\partial q_l} \left(\frac{\partial x_k}{\partial t} + \sum_m \frac{\partial x_k}{\partial q_m} \dot{q}_m \right) = \frac{\partial}{\partial q_l} \frac{dx_k}{dt} = \frac{\partial \dot{x}_k}{\partial q_l} \tag{213}$$

With this, also the second term on the right side in (212) vanishes, and the Euler-Lagrange equations in the new coordinates $\{q_l\}$ and the corresponding velocities are recovered.

6.2.4 Generalized momenta and cyclic coordinates

Newton's laws made an explicit statement on the quantity momentum associated with a Cartesian coordinate x_k , defined in (150) as $p_k = m_k \dot{x}_k$. To come to a similarly useful definition for generalized coordinates, we first try to extract the linear momentum p_k from the Lagrange function. We first note that the required velocity \dot{x}_k appears in the expression (149) of the kinetic energy,

$$T = \sum_{k} \frac{1}{2} m_k \dot{x}_k^2 \,. \tag{214}$$

The momentum p_k can be extracted from T by differentiating with respect to \dot{x}_k :

$$\frac{\partial T}{\partial \dot{x}_k} = m_k \dot{x}_k = p_k \tag{215}$$

Since Lagrange function is the difference between T and a potential U that should not depend on the velocities, one can obtain the momentum directly by differentiating the Lagrange function with respect to \dot{x}_k . This can be used to define a generalized momentum, if the Lagrange function is expressed in generalized coordinates $\{q_l\}$ and generalized velocities $\{\dot{q}_l\}$:

$$p_k := \frac{\partial L}{\partial \dot{q}_k} \tag{216}$$

The difference between generalized momentum and the traditional momentum can e.g. be seen with the Lagrange function of a charged particle in an electromagnetic field from (166):

$$L = \sum_{i=1}^{3} \frac{1}{2} m \dot{x}_i^2 - q \Phi(\mathbf{x}) + \sum_{i=1}^{3} q \dot{x}_i A_i(\mathbf{x}).$$
 (217)

The corresponding generalized momentum to the coordinate x_i is

$$p_i = \frac{\partial L}{\partial \dot{x}_i} = m\dot{x}_i + qA_i(\mathbf{x}), \qquad (218)$$

which contains not only the kinetic momentum $m\dot{x}_i$ of the particle's motion, but also a contribution qA_i from the vector potential.

The generalized momentum can also be used to rewrite the Euler-Lagrange equation:

$$\frac{\partial L}{\partial q_k} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_k} = \frac{\partial L}{\partial q_k} - \frac{d}{dt} p_k = 0 \quad \text{or} \quad \dot{p}_k = \frac{\partial L}{\partial q_k}$$
 (219)

This has an important consequence if the Lagrange function does not depend on a particular generalized coordinate q_k . Such coordinates are called *cyclic*. If q_k is a cyclic coordinate, $\partial L/\partial q_k = 0$, and

$$\dot{p}_k = 0 \quad \text{or} \quad p_k = const. \tag{220}$$

So if L does not depend on a coordinate q_k , and is therefore symmetric with respect to a translation in q_k , the corresponding generalized momentum does not change in time or is *conserved*.

We will expand more on this important connection between symmetries and conserved quantities that holds for any generalized coordinate and its canonically conjugated momentum, because it will help to explore symmetries in problems.

6.3 Noether's theorem: Symmetries and conservation laws

The conservation of the canonically conjugated momentum of a cyclic generalized coordinate deserves slightly more attention, because it can be expanded to different symmetries. The mathematically rigorous version of this idea was formulated by Emmy Noether⁷, and the connection between symmetries and conserved quantities is known as the *Noether theorem*. In a simple form of this theorem, symmetries are expressed as an invariance of the Lagrange function against small symmetry transformations. Here, we consider three different symmetry examples: translation symmetry in space, rotation symmetry, and translation symmetry in time. However, this is a very general principle that reaches way beyond classical mechanics, and is e.g. heavily used in elementary particle physics.

6.3.1 Translation symmetry and momentum conservation

If a Lagrangian does not explicitly depend on a particular coordinate q_k , i.e., q_k is cyclic, L is symmetric with respect to a translation in this coordinate; this caused momentum conservation (220).

We now use a slightly different way of noting this symmetry that will allow treating the rotational symmetry easier later. First, we consider a transformation

$$\mathbf{q} \to \mathbf{q'} = \mathbf{q} + \delta \mathbf{q} \,, \tag{221}$$

where \mathbf{q} is a vector of (generalized) coordinates, and $\delta \mathbf{q}$ a small displacement vector in a particular direction. We can decompose this displacement with the help of a unit vector set $\{\mathbf{e}_l\}$:

$$\delta \mathbf{q} = \sum_{l} \delta q_{l} \, \mathbf{e}_{l} \,, \tag{222}$$

with small time-independent displacements δq_l . Then, the change δL of the Lagrange function under such a transformation is given by

$$\delta L = \sum_{l} \left(\frac{\partial L}{\partial q_{l}} \delta q_{l} + \frac{\partial L}{\partial \dot{q}_{l}} \delta \dot{q}_{l} \right) . \tag{223}$$

The last term vanishes, as $\delta \dot{q}_l = d(\delta q_l)/dt$ and the small displacements δ_l do not depend on time. A symmetry with respect to a small translation means that the Lagrange function should not change under this transformation, or $\delta L = 0$. Thus,

$$\delta L = \sum_{l} \frac{\partial L}{\partial q_{l}} \delta q_{l} = \sum_{l} \dot{p}_{l} \delta q_{l} = \dot{\mathbf{p}} \cdot \delta \mathbf{q} = 0.$$
 (224)

We can interpret this result in the following way: if the system (and therefore the Lagrangian) has a translational symmetry in the direction $\delta \mathbf{q}$, the *projection* of the generalized momentum \mathbf{p} on this direction does not change in time, or is conserved.

⁷A. Emmy Noether, 1882-1935

6.3.2 Rotational symmetry and angular momentum conservation

We recall from section 1.5 that infinitesimal rotations can be described by a vector $\delta \boldsymbol{\theta}$, which according to (44) causes a displacement of something at position \mathbf{r} (referenced to a point on the rotation axis) by

$$\delta \mathbf{r} = \delta \boldsymbol{\theta} \times \mathbf{r}$$
, and also $\delta \dot{\mathbf{r}} = \delta \boldsymbol{\theta} \times \dot{\mathbf{r}}$ (225)

because the vector $\delta \boldsymbol{\theta}$ should not depend on time. Under this position transformation

$$\mathbf{r} \to \mathbf{r}' = \mathbf{r} + \delta \mathbf{r}$$
, (226)

the change of the Lagrange function is given by

$$\delta L = \sum_{l=1}^{3} \left(\underbrace{\frac{\partial L}{\partial x_{l}}}_{=\dot{p}_{l}} \delta x_{l} + \underbrace{\frac{\partial L}{\partial \dot{x}_{l}}}_{=p_{l}} \delta \dot{x}_{l} \right)$$

$$= \sum_{l=1}^{3} \dot{p}_{l} \delta x_{l} + p_{l} \delta \dot{x}_{l}$$

$$= \dot{\mathbf{p}} \cdot \delta \mathbf{r} + \mathbf{p} \cdot \delta \dot{\mathbf{r}} = \dot{\mathbf{p}} \cdot (\delta \boldsymbol{\theta} \times \mathbf{r}) + \mathbf{p} \cdot (\delta \boldsymbol{\theta} \times \dot{\mathbf{r}}). \tag{227}$$

With the cyclic permutation symmetry of the triple product⁸ $\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \mathbf{b} \cdot (\mathbf{c} \times \mathbf{a})$,

$$\delta L = \delta \boldsymbol{\theta} \cdot (\mathbf{r} \times \dot{\mathbf{p}}) + \delta \boldsymbol{\theta} \cdot (\dot{\mathbf{r}} \times \mathbf{p})
= \delta \boldsymbol{\theta} \cdot (\mathbf{r} \times \dot{\mathbf{p}} + \dot{\mathbf{r}} \times \mathbf{p})
= \delta \boldsymbol{\theta} \cdot \left(\frac{d}{dt} (\mathbf{r} \times \mathbf{p})\right)
= \delta \boldsymbol{\theta} \cdot \dot{\mathbf{L}},$$
(228)

where **L** was the angular momentum vector introduced in (73). If the physical system is symmetric with respect to a rotation defined by $\delta \theta$, the Lagrangian does not change, i.e., δL =0. Then,

$$\delta \boldsymbol{\theta} \cdot \dot{\mathbf{L}} = 0, \tag{229}$$

which means that the projection of the angular momentum vector \mathbf{L} on the axis of rotational symmetry, defined by the direction of $\boldsymbol{\theta}$, is a constant in time, or is conserved. An example would be a spherical pendulum, where a mass m suspended by a string of length l in gravity is allowed oscillating freely. We leave it to the reader to work out the Lagrange function for that case, but it should be obvious that neither the potential nor the kinetic energy depend on the polar

⁸The product $\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})$ is used to calculate the volume of a parallelepiped spanned by the three vectors \mathbf{a} , \mathbf{b} , and \mathbf{c} .

angle, thus the angular momentum component along the vertical direction is conserved.

For a spherically symmetric problem, the Lagrangian is independent of rotations around all directions in space, thus, all components of the angular momentum are conserved.

6.3.3 Invariance against translation in time and energy conservation

We now consider a different symmetry, where the physical system is invariant by a translation in time:

$$t \to t' = t + \delta t \,. \tag{230}$$

Then, the change of the Lagrangian under small changes δt must vanish, or

$$\frac{\partial L}{\partial t} = 0, (231)$$

i.e., the Lagrange function is not explicitly time dependent. Under this condition, we can calculate the total differential of the Lagrange function with respect to time (because the system can still evolve, causing L to change over time):

$$\frac{d}{dt}L = \sum_{k} \left(\frac{\partial L}{\partial q_{k}} \dot{q}_{k} + \frac{\partial L}{\partial \dot{q}_{k}} \ddot{q}_{k} \right)$$

$$= \sum_{k} \left(\left[\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_{k}} \right) \right] \dot{q}_{k} + \frac{\partial L}{\partial \dot{q}_{k}} \ddot{q}_{k} \right)$$

$$= \sum_{k} \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_{k}} \dot{q}_{k} \right) \tag{232}$$

From the first line to the second, the Lagrange equation (153) allows replacing $\partial L/\partial q_k$, and from the second to third line, the product rule for differentiations was applied. The differentiation with respect to time in the last line can be taken out of the sum, and the whole equation (232) can be written as

$$\frac{d}{dt}\left(\sum_{k} \frac{\partial L}{\partial \dot{q}_{k}} \dot{q}_{k} - L\right) = 0 \quad \text{or} \quad \frac{d}{dt}H = 0 \tag{233}$$

The quantity in the parenthesis above is defined as the *Hamilton function*

$$H := \sum_{k} \frac{\partial L}{\partial \dot{q}_{k}} \dot{q}_{k} - L \tag{234}$$

of the problem, and is constant in time, or conserved if the physical system and therefore the Lagrangian is symmetric with respect to a translation in time. In many cases, the Hamilton function is the same as the total energy. In those cases, the invariance of L under translations in time means that the total energy

of the system is conserved, as we have seen in section 3.3 and 4.5. Equation (233) expresses energy conservation for a physical system described in *generalized* coordinates, but with the same assumption on the time-independence of U as earlier. To identify H with the total energy E, there is another constraint to consider in how the generalized coordinates are connected with the Cartesian coordinates.

6.4 Hamilton function and total energy

To interpret the Hamilton function defined in (234), we detour to an aspect of the total kinetic energy T of the system. In Cartesian coordinates, the kinetic energy can be written as

$$T = \sum_{k} \frac{1}{2} m_k \dot{x}_k^2 \,. \tag{235}$$

Via the point transformations (207) between $\{x_k\}$ and $\{q_l\}$, and using (208), the kinetic energy can be expressed via generalized velocities \dot{q}_l :

$$T = \sum_{k} \frac{1}{2} m_{k} \left(\sum_{l} \frac{\partial x_{k}}{\partial q_{l}} \dot{q}_{l} + \frac{\partial x_{k}}{\partial t} \right) \left(\sum_{l'} \frac{\partial x_{k}}{\partial q_{l'}} \dot{q}_{l'} + \frac{\partial x_{k}}{\partial t} \right)$$

$$= \sum_{l,l'} \left[\sum_{k} \frac{1}{2} m_{k} \frac{\partial x_{k}}{\partial q_{l}} \frac{\partial x_{k}}{\partial q_{l'}} \right] \dot{q}_{l} \dot{q}_{l'} + \sum_{l} \left[2 \sum_{k} \frac{1}{2} m_{k} \frac{\partial x_{k}}{\partial q_{l}} \frac{\partial x_{k}}{\partial t} \right] \dot{q}_{l} + \left[\sum_{k} \frac{1}{2} m_{k} \left(\frac{\partial x_{k}}{\partial t} \right)^{2} \right]$$

$$= \sum_{l,l'} a_{l,l'} \dot{q}_{l} \dot{q}_{l'} + \sum_{l} b_{l} \dot{q}_{l} + c, \qquad (236)$$

where $a_{l,l'}$, b_l , and c summarize the corresponding brackets in the line before. For time-independent point transformations from $\{x_k\}$ to generalized coordinates $\{q_l\}$,

$$\frac{\partial x_k}{\partial t} = 0, (237)$$

so $b_l = c = 0$ in the kinetic energy expression (236), which then simplifies to

$$T = \sum_{l,l'} a_{l,l'} \, \dot{q}_l \dot{q}_{l'} \,. \tag{238}$$

Then, the partial derivative of T with respect to velocities \dot{q}_k are

$$\frac{\partial T}{\partial \dot{q}_k} = \sum_{l} a_{l,k} \, \dot{q}_l + \sum_{l'} a_{k,l'} \, \dot{q}_{l'} = \sum_{l} (a_{l,k} + a_{k,l}) \, \dot{q}_l \tag{239}$$

In the first step, the two terms appear because in the double sum in (238), \dot{q}_k appears twice. In the second step, a variable change $l' \to l$ for the sum allowed taking everything under one sum. With this, one can evaluate the following sum:

$$\sum_{k} \dot{q}_{k} \frac{\partial T}{\partial \dot{q}_{k}} = \sum_{k,l} (a_{l,k} + a_{k,l}) \dot{q}_{k} \dot{q}_{l}$$

$$= 2 \sum_{k,l} a_{l,k} \dot{q}_{k} \dot{q}_{l} = 2T.$$
(240)

The step from the first to the second line simply involved a summation index exchange $k \leftrightarrow l$ for one of the sums.

The relation (240) is special case of a property of so-called *homogenous functions*. A multi-variable function $f(\lbrace q_k \rbrace)$ is called homogenous of degree p, if

$$f(\{\lambda q_k\}) = \lambda^p f(\{q_k\}). \tag{241}$$

This means that if all parameters of f are multiplied by a constant λ , the value of f is the value of the original function, multiplied with λ^p . For example, the function $f(x,y) = x^2 + y^2$ is homogenous of degree p = 2 in x, y. For homogenous functions, Euler⁹ showed that

$$\sum_{k} q_k \frac{\partial f}{\partial q_k} = pf \,, \tag{242}$$

which is referred to as Euler's theorem on homogenous functions.

After this small detour, we come back to the definition of the Hamilton function (234). If we assume that the potential U in L = T - U is independent of the velocities \dot{q}_k , then

$$\frac{\partial L}{\partial \dot{q}_k} = \frac{\partial T}{\partial \dot{q}_k} \,, \tag{243}$$

and we can write

$$H = \sum_{k} \frac{\partial L}{\partial \dot{q}_{k}} \dot{q}_{k} - L$$

$$= \sum_{k} \frac{\partial T}{\partial \dot{q}_{k}} \dot{q}_{k} - L = 2T - L = 2T - (T - U) = T + U \qquad (244)$$

So the Hamilton function becomes the total energy (i.e., the sum of total kinetic and potential energy) under the assumptions we made when interpreting H. Explicitly, these assumptions were

- (a) the transformations form Cartesian to generalized coordinates $\{q_k\}$ used as parameters for L and H are time-independent, and
- (b) the potential energy U is independent of the velocities \dot{q}_k .

An example where $H \neq E$ can be found with rotating coordinate systems, since this makes the coordinate transformations to a inertial reference frame timedependent. Still, the total energy may be conserved.

⁹Leonhard Euler, 1707-1783

6.5 Non-conservative forces in the Lagrange formalism

So far, the description of physical systems by the Euler-Lagrange formalism required that forces can be expressed as a gradient of a potential, and do not depend velocities, with notable exceptions like charged particles in electromagnetic fields in section 5.2. However, friction forces and other dissipative forces that can not be expressed by a potential or a Lagrange function are an important part of many practical systems, so a mechanism to include these phenomena in the very flexible Lagrange formalism is desirable.

To do this, we recall the definition of the work integral (130) in section 4.3, where the work on an ensemble of particles transitioning from state a to b was defined as

$$W_{ab} = \sum_{\alpha} \int_{a}^{b} \mathbf{F}_{\alpha} \cdot d\mathbf{x}_{\alpha} \,. \tag{245}$$

The position \mathbf{x}_{α} of particle α can be expressed by generalized coordinates,

$$\mathbf{x}_{\alpha} = \mathbf{x}_{\alpha}(\{q_k\}), \tag{246}$$

as long as the transformation between real and generalized coordinates is not explicitly time dependent. The differential displacement $d\mathbf{x}_{\alpha}$ can be written

$$d\mathbf{x}_{\alpha} = \sum_{k} \frac{\partial \mathbf{x}_{\alpha}}{\partial q_{k}} \, dq_{k} \,, \tag{247}$$

and the differential dW for the total work on the system by the forces \mathbf{F}_{α} is

$$dW = \sum_{\alpha} \mathbf{F}_{\alpha} \cdot d\mathbf{x}_{\alpha}$$

$$= \sum_{\alpha,k} \mathbf{F}_{\alpha} \cdot \left(\frac{\partial \mathbf{x}_{\alpha}}{\partial q_{k}}\right) dq_{k}$$

$$= \sum_{k} \phi_{k} dq_{k}, \qquad (248)$$

with the definition of the so-called *generalized* force

$$\phi_k := \sum_{\alpha} \mathbf{F}_{\alpha} \cdot \frac{\partial \mathbf{x}_{\alpha}}{\partial q_k} \,. \tag{249}$$

Expression (248) holds for any type of force, and we now try to reproduce the Lagrange equations. For that, we start with the expression for the total kinetic energy as expressed by Cartesian velocities,

$$T = \sum_{\alpha} \frac{1}{2} m_{\alpha} (\dot{\mathbf{x}}_{\alpha})^2 \,, \tag{250}$$

and calculate their derivatives with respect to generalized coordinates q_k :

$$\frac{\partial T}{\partial q_k} = \sum_{\alpha} m_{\alpha} \,\dot{\mathbf{x}}_{\alpha} \cdot \frac{\partial \dot{\mathbf{x}}_{\alpha}}{\partial q_k} \tag{251}$$

From (247), one finds

$$\dot{\mathbf{x}}_{\alpha} = \sum_{k} \frac{\partial \mathbf{x}_{\alpha}}{\partial q_{k}} \dot{q}_{k}$$
 and thus $\frac{\partial \dot{\mathbf{x}}_{\alpha}}{\partial \dot{q}_{k}} = \frac{\partial \mathbf{x}_{\alpha}}{\partial q_{k}}$ (252)

With this, the derivative of the kinetic energy with respect to the generalized velocity \dot{q}_k is

$$\frac{\partial T}{\partial \dot{q}_k} = \sum_{\alpha} m_{\alpha} \, \dot{\mathbf{x}}_{\alpha} \cdot \frac{\partial \dot{\mathbf{x}}_{\alpha}}{\dot{q}_k} = \sum_{\alpha} m_{\alpha} \, \dot{\mathbf{x}}_{\alpha} \cdot \frac{\partial \mathbf{x}_{\alpha}}{\partial q_k} \,. \tag{253}$$

This allows assembling the kinetic energy dependent part of a Lagrange equation:

$$\frac{\partial T}{\partial q_k} - \frac{d}{dt} \frac{\partial T}{\partial \dot{q}_k} = \sum_{\alpha} m_{\alpha} \dot{\mathbf{x}}_{\alpha} \cdot \frac{\partial \dot{\mathbf{x}}_{\alpha}}{\partial q_k} - \frac{d}{dt} \left(\sum_{\alpha} m_{\alpha} \dot{\mathbf{x}}_{\alpha} \cdot \frac{\partial \mathbf{x}_{\alpha}}{\partial q_k} \right)
= \sum_{\alpha} m_{\alpha} \left[\dot{\mathbf{x}}_{\alpha} \cdot \frac{\partial \dot{\mathbf{x}}_{\alpha}}{\partial q_k} - \ddot{\mathbf{x}}_{\alpha} \cdot \frac{\partial \mathbf{x}_{\alpha}}{\partial q_k} - \dot{\mathbf{x}}_{\alpha} \cdot \frac{d}{dt} \frac{\partial \mathbf{x}_{\alpha}}{\partial q_k} \right]
= -\sum_{\alpha} m_{\alpha} \ddot{\mathbf{x}}_{\alpha} \cdot \frac{\partial \mathbf{x}_{\alpha}}{\partial q_k}.$$
(254)

Using Newton's equation of motion $\mathbf{F}_{\alpha} = m_{\alpha} \ddot{\mathbf{x}}_{\alpha}$ and the definition (249) for the generalized force, one obtains

$$\frac{\partial T}{\partial q_k} - \frac{d}{dt} \frac{\partial T}{\partial \dot{q}_k} = -\sum_{\alpha} \mathbf{F}_{\alpha} \cdot \frac{\partial \mathbf{x}_{\alpha}}{\partial q_k} = -\phi_k.$$
 (255)

The generalized force can always be split up in a part that can be derived from a potential U, and a residual part ϕ'_k ,

$$\phi_k = -\frac{\partial U}{\partial q_k} + \phi_k', \qquad (256)$$

with a velocity-independent potential $U = U(\lbrace q_k \rbrace)$. Then, the equation of motion (255) can be written as

$$\frac{\partial (T-U)}{\partial q_k} - \frac{d}{dt} \frac{\partial (T-U)}{\partial \dot{q}_k} = \frac{\partial L}{\partial q_k} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_k} = -\phi_k', \qquad (257)$$

where L=T-U is the usual Lagrange function that contains forces that can be derived from a potential. Expression (257) resembles almost the set of Lagrange equations (206), but this time, non-conservative forces like the friction forces seen in section 2.3.2 can be taken into account as well. If there are no dissipative forces, $\phi_k'=0$, and the original Euler-Lagrange equations (206) are reproduced.

The strategy to handle problems with such forces would be as follows: First, formulate a Lagrange function L with the kinetic energy and the potential from interactions or forces that can be expressed via a potential U in convenient coordinates. Then, evaluate the generalized forces ϕ'_k for the non-conservative forces from their description in real space via (249). Subsequently, solve the set of (possibly coupled) differential equations (257).

6.6 Constraints in the Lagrange formalism

One of the advantages of the Lagrange formalism is that constraints in the motion of particles can be elegantly taken care of by an adequate choice of coordinates. In an adequate coordinate system, a constraint does not explicitly not show up in the equation of motion, and the number of degrees of freedoms or generalized coordinates q_k is reduced by the number of constraints.

Sometimes, however, it may be better to keep more generalized coordinates in the system of differential equations to be solved. There is a specific method within the Euler-Lagrange formalism that can handle explicit constraints.

Constraints between a set of coordinates are typically formulated in the form

$$f(\{q_k\}) = 0. (258)$$

An example would be the motion of a point mass on the surface of a sphere in the usual three-dimensional space with coordinates x, y and z. There, the constraint to the surface of a sphere with radius r is

$$f(x, y, x) = x^{2} + y^{2} + z^{2} - r^{2} = 0.$$
 (259)

In general, constraints can not only be a function of coordinates q_k , but also a function of the velocities \dot{q}_k , or explicitly the time t. The constraints are typically classified into the following categories:

	scleronomic (fixed in time)	rheonomic (time-dependent)
holonomic (independent of \dot{q}_k)	$f(\{q_k\}) = 0$	$f(\{q_k\},t)=0$
non-holonomic (dependent on \dot{q}_k)	$f(\{q_k\},\{\dot{q}_k\})=0$	$f(\{q_k\}, \{\dot{q}_k\}, t) = 0$

The method of *undetermined Lagrange multipliers* allows taking care of holonomic constraints, and certain non-holonomic constraints if they are of a certain form.

To see how these can be taken care of, we recall the variational problem in section 6.1, and formulate it for two variables y and z that are connected via a constraint

$$g(y, z; x) = 0. (260)$$

As a reminder, in the Euler problem for the case at hand we were looking for solutions y(x) and z(x) which make the functional

$$J = \int_{x_1}^{x_2} f(y, y', z, z'; x) dx$$
 (261)

extremal (i.e., minimal or maximal). This was done by adding deviations η_i with a control parameter α to the desired solutions,

$$y(\alpha, x) = y(x) + \alpha \eta_1(x), \quad z(\alpha, x) = z(x) + \alpha \eta_2(x). \tag{262}$$

The extremal condition for J according to (191) for the two functions y and z is then explicitly

$$\frac{\partial J}{\partial \alpha} = \int_{x_1}^{x_2} \left[\left(\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y'} \right) \frac{\partial y}{\partial \alpha} + \left(\frac{\partial f}{\partial z} - \frac{d}{dx} \frac{\partial f}{\partial z'} \right) \frac{\partial z}{\partial \alpha} \right] dx \stackrel{!}{=} 0, \quad (263)$$

where the derivatives of y and z with respect to α are the deviation functions $\eta_i(x)$ from the optimal path:

$$\eta_1(x) = \frac{\partial y}{\partial \alpha} \quad \text{and} \quad \eta_2(x) = \frac{\partial z}{\partial \alpha}.$$
(264)

As $\partial J/\partial \alpha = 0$ needed to be valid for all possible independent deviations $\eta_i(x)$, it was necessary that both parentheses in (263) are vanishing identically, which led to the Euler equations for y and z. With constraint (260), however, the deviations are not independent anymore, but connected via

$$\frac{dg}{d\alpha} = \frac{\partial g}{\partial y}\frac{\partial y}{\partial \alpha} + \frac{\partial g}{\partial z}\frac{\partial z}{\partial \alpha} = \frac{\partial g}{\partial y}\eta_1 + \frac{\partial g}{\partial z}\eta_2 = 0.$$
 (265)

The deviation η_2 now can be expressed via the deviation η_1 ,

$$\eta_2 = -\eta_1 \frac{\partial g/\partial y}{\partial g/\partial z}, \qquad (266)$$

so the condition for an extremal J turns into

$$\frac{\partial J}{\partial \alpha} = \int_{x_1}^{x_2} \left[\left(\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y'} \right) - \left(\frac{\partial f}{\partial z} - \frac{d}{dx} \frac{\partial f}{\partial z'} \right) \frac{\partial g/\partial y}{\partial g/\partial z} \right] \eta_1(x) dx \stackrel{!}{=} 0.$$
 (267)

For this expression to hold for all deviations $\eta_1(x)$, the square bracket needs to vanish identically, or

$$\left(\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y'}\right)\frac{1}{\partial g/\partial y} = \left(\frac{\partial f}{\partial z} - \frac{d}{dx}\frac{\partial f}{\partial z'}\right)\frac{1}{\partial g/\partial z} =: -\lambda.$$
(268)

As each side of this expression contains derivatives with respect to y and y', or z and z' only, the so-called Lagrange undetermined multiplier λ can at most be a function of x. Then,

$$\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y'} + \lambda(x) \frac{\partial g}{\partial y} = 0, \text{ and}$$

$$\frac{\partial f}{\partial z} - \frac{d}{dx} \frac{\partial f}{\partial z'} + \lambda(x) \frac{\partial g}{\partial z} = 0.$$
(269)

This is a set of differential equations for three functions y(x), z(x) and $\lambda(x)$. Together with the constraint condition (260), there are three equations for the three unknown functions.

The method can be extended to more than two functions, and more than a single constraint. Applying this general formalism to the Hamilton principle, the Euler-Lagrange equations of motion with s constraints become

$$\frac{\partial L}{\partial q_k} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_k} + \sum_{i=1}^s \lambda_i(t) \frac{\partial f_i}{\partial q_k} = 0, \qquad (270)$$

with s constraint equations $f_i = 0$ for the dynamic variables $q_k(t)$, and the s Lagrange undetermined multipliers $\lambda_i(t)$.

Comparing (270) with the definition of equations of motion under arbitrary generalized forces in (257), one can interpret the Lagrange multipliers directly as forces that are not captured by standard Lagrange formalism:

$$\frac{\partial L}{\partial q_k} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_k} = -\sum_{i=1}^s \lambda_i(t) \frac{\partial f_i}{\partial q_k} = -\sum_{i=1}^s \phi_{i,k} \quad \text{with} \quad \phi_{i,k} := \lambda_i(t) \frac{\partial f_i}{\partial q_k}. \quad (271)$$

The $\phi_{i,k}$ represents the constraining force in direction of coordinate q_k due to the constraint $f_i = 0$. This is useful to find out the constraining forces in the Lagrange formalism, which tries to avoid the calculation of constraining forces by an adequate choice of variables to describe the problem. Such constraining forces are not interesting to understand the dynamics of the system, but may be important in an "engineering" context, where a system has to be designed to provide the constraining forces.

7 Elements of Hamiltonian mechanics

The introduction of the Hamilton function has a much wider use than that of a conserved quantity in time-invariant physical systems. In a similar way as the Lagrange function is used to derive the complete dynamics of a system, there is a method constructing a set of equations of motion that are based on the Hamilton function. This method offers some advantages in the complexity of the equation of motion, and may lead to a better handling of cyclic variables. The main advantage of that method, however, is in its use in other areas of physics, namely quantum mechanics: There, the Hamilton function is at the center of describing the dynamics of a system. Similarly, Hamiltonian mechanics is heavily used is in statistical physics, when ensembles of many particles, like in a fluid, are analyzed.

The starting point for this yet another approach to find equations of motion of a system is the transition from a dynamic variable set $\{q_k, \dot{q}_k\}$ to a set that is made up by the generalized coordinates, and their canonically conjugated momenta, $\{q_k, p_k\}$. This should be possible because the momenta p_k and velocities \dot{x}_k carry somewhat similar information.

We remember the definition (216) of the generalized momentum,

$$p_k = \frac{\partial L}{\partial \dot{q}_k} \tag{272}$$

and also write the Lagrange equations of motion (153) with this momentum:

$$\frac{\partial L}{\partial q_k} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_k} = 0 \quad \to \quad \dot{p}_k = \frac{\partial L}{\partial q_k}$$
 (273)

A fast way to come to equations of motion is to write the Hamilton function as a function of the new dynamic variables (and time, if necessary):

$$H = H(\{q_k\}, \{p_k\}, t), \qquad (274)$$

and try to write down the full differential dH in all the variables:

$$dH = \sum_{k} \left(\frac{\partial H}{\partial q_k} dq_k + \frac{\partial H}{\partial p_k} dp_k \right) + \frac{\partial H}{\partial t} dt.$$
 (275)

In a next step, we try to express the total differential dH from its definition (234), and identify the partial derivatives in (275). For this, we first simplify the Hamilton function by using definition of p_k ,

$$H = \sum_{k} \frac{\partial L}{\partial \dot{q}_{k}} \dot{q}_{k} - L = \sum_{k} p_{k} \dot{q}_{k} - L, \qquad (276)$$

and then calculate the total differential dH from this expression:

$$dH = d(\sum_{k} p_k \, \dot{q}_k - L) = d \sum_{k} p_k \, \dot{q}_k - dL$$

$$= \sum_{k} (p_{k} d\dot{q}_{k} + \dot{q}_{k} dp_{k}) - \left[\sum_{k} \underbrace{\frac{\partial L}{\partial q_{k}}}_{=\dot{p}_{k}} dq_{k} + \underbrace{\frac{\partial L}{\partial \dot{q}_{k}}}_{=p_{k}} d\dot{q}_{k} + \frac{\partial L}{\partial t} dt \right]$$

$$= \sum_{k} (p_{k} d\dot{q}_{k} + \dot{q}_{k} dp_{k} - \dot{p}_{k} dq_{k} - p_{k} d\dot{q}_{k}) - \frac{\partial L}{\partial t} dt$$

$$= \sum_{k} (\dot{q}_{k} dp_{k} - \dot{p}_{k} dq_{k}) - \frac{\partial L}{\partial t} dt$$

$$(277)$$

In this transformation, the Lagrange equation of motion was inserted when $\partial L/\partial q_k$ was replaced with \dot{p}_k . The result is a full differential dH, expressed in full differentials of the parameters of H. By comparing the coefficients in (275) and (277), one finds

$$\dot{q}_k = \frac{\partial H}{\partial p_k}, \qquad -\dot{p}_k = \frac{\partial H}{\partial q_k},$$
 (278)

and

$$-\frac{\partial L}{\partial t} = \frac{\partial H}{\partial t} \,. \tag{279}$$

Equations (278) are in fact already the equations of motion for the dynamic variables q_k and p_k , and are referred to as *Hamilton's equation of motion*.

If there are N degrees of freedom (i. e., N different indices k), then (278) forms a system of 2N ordinary differential equations of first order. They are equivalent with the other equations of motion of a system; the Lagrange equations of motion (153) form a system of N differential equations of second order. Both sets of equations of motion require 2N integration constants to be solved.

Before we use the Hamiltonian approach, we look at the total temporal derivative of the Hamilton function, which was shown to vanish if a system was invariant to translations in time (see section 6.3.3). It can be directly calculated:

$$\dot{H} = \frac{dH}{dt} = \sum_{k} \left(\frac{\partial H}{\partial q_{k}} \dot{q}_{k} + \frac{\partial H}{\partial p_{k}} \dot{p}_{k} \right) + \frac{\partial H}{\partial t}$$

$$= \sum_{k} \left(-\dot{p}_{k} \dot{q}_{k} + \dot{q}_{k} \dot{p}_{k} \right) + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t} . \tag{280}$$

The total derivative H is the same as the explicit time dependency $\partial H/\partial t$, so if H is not explicitly time dependent, H is a conserved quantity. As before, if U is independent of the velocities \dot{q}_k , and the transformations from $\{x_l\}$ to $\{q_k\}$ is independent of time, then H = E.

The strategy to obtain the Hamilton equations of motion is summarized below:

- 1. Express the kinetic energy T in the velocities \dot{q} .
- 2. Find the potential energy U as a function of the coordinates q_k .

- 3. Find the canonically conjugated momenta $p_k = \partial L/\partial \dot{q}_k$
- 4a. Express the kinetic energy T in these momenta p_k if this is easy, and obtain the Hamilton function H = T + U directly if the conditions for H = E are met (no time-dependent coordinates q_k , no \dot{q}_k in U).
- 4b. Otherwise, obtain H via the definition (234).
- 5. Proceed to the equations of motion (278).

7.1 Simple example: harmonic oscillator

As before, we apply the Hamiltonian formalism first to a simple physical system, the one-dimensional harmonic oscillator. We have seen in section 5.1 that

$$T = \frac{1}{2}m\dot{x}^2$$
 and $U = \frac{1}{2}kx^2$. (281)

We use the standard Cartesian coordinate x as coordinate, and find the corresponding momentum

$$p = \frac{\partial L}{\partial \dot{x}} = \frac{\partial (T - U)}{\partial \dot{x}} = \frac{\partial T}{\partial \dot{x}} = m\dot{x}.$$
 (282)

This allows expressing the kinetic energy via the momentum,

$$T = \frac{p^2}{2m},\tag{283}$$

and since U is not velocity-dependent and we work with Cartesian coordinates,

$$H = T + U = \frac{p^2}{2m} + \frac{kx^2}{2} \,. \tag{284}$$

The resulting set of equations of motion obtained via (278) is then

$$\dot{x} = \frac{1}{m} p$$
, and $\dot{p} = -kx$. (285)

For this simple example, the two equations of motion can not be solved easier than it used to be before, as both differential equations are coupled.

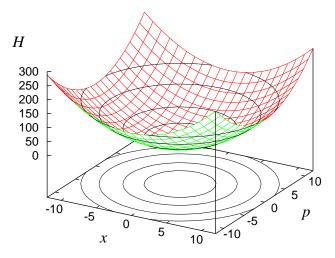
The advantages of this formalism come really out on more complex problems, where several coordinates are cyclic.

7.2 Hamilton dynamics and phase space

The transition to dynamic variables $\{q_k\}$ and $\{p_k\}$ allows visualizing the trajectory of a system in this so-called *phase space*. To do so, we first keep in mind that for many systems, the Hamilton function H is a constant in time. Therefore, in a diagram that represents the function $H(\{q_k\}, \{p_k\})$, the trajectory of the system moves along a line of constant H. For example, the Hamiltonian of the harmonic oscillator had a parabolic shape in x and p,

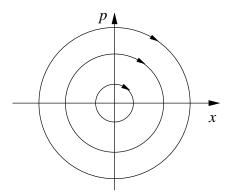
$$H = T + U = \frac{p^2}{2m} + \frac{kx^2}{2}, \qquad (286)$$

and the contour lines for a constant energy E (shown in black below) are ellipses:

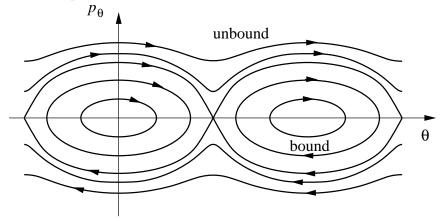


In an appropriate scaling, the time evolution of the harmonic oscillator is just a rotation in phase space around the origin, with a constant angular frequency $\omega = \sqrt{k/m}$, independent of the amplitude of the oscillation, and the trajectories in phase space are closed after a period $T = 2\pi/\omega$:

Similarly to the simple picture where qualitative statements could be made on a solution by knowing the potential energy in section 3.3.1, statements can be made from observing contours with fixed total energy in phase space. First, it allows identifying the type of solutions one can expect: If the plane of a constant energy cuts the Hamilton function near a local minimum in phase space, the trajectory in phase space will be closed loops, pretty much as shown in the graphics above. But for higher energies, there may be solutions that are not bound - the plane pendulum (see section 6.2.1) with coordinate θ would be such an example, where



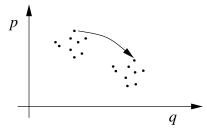
there are oscillatory solutions as well as solutions that increase θ monotonously in time when the pendulum rotates:



For a given total energy E, some statements about maximal and minimal angles θ can be made, or for maximal and minimal values for the corresponding generalized momentum p_{θ} (which happens to be the angular momentum).

7.3 Hamiltonian mechanics for an ensemble of systems

The concept of phase space becomes very useful if a physical system is obeyed in the same way by a large number of particles, like molecules in a gas. Then, the different systems can be represented by a point moving in the same phase space at once, and one can ask the question of how an ensemble of system distributes over time:



The ensemble will move in a particular way, but the arrangement of points in

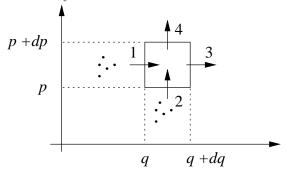
phase space may change its shape or orientation over time. In such a situation, it can be useful to introduce a density ρ of systems in phase space, that describes how many systems dN can be found in a infinitesimal phase space volume dv:

$$dN = \rho dv, \qquad (287)$$

where dv is a volume in a phase space for the s coordinate/momentum pairs:

$$dv = (dq_1 dq_2 \cdots dq_s)(dp_1 dp_2 \cdots dp_s). \tag{288}$$

For a small volume element in phase space, one can balance how many systems enter and leave the volume in a timer interval dt. For this purpose, we consider the small area dq dp in the in the phase space for one coordinate q and momentum p, and evaluate the flow of systems into this area:



The number of systems dN_1 that enter the volume in the time interval dt (or the rate dN_1/dt) from the left is

$$\frac{dN_1}{dt} = \rho \frac{dq}{dt} dp = \rho \dot{q} dp. \tag{289}$$

This can be understood in the following way: The first term ρ measures how many points are there per unit phase space area, the second term \dot{q} captures how fast these points move from left to right into the volume, and the third term dp captures how wide the area is in p direction where systems can enter the area under consideration. The expression $\rho \dot{q}$ is therefore a flow density per unit of p. In a similar way, the rate of systems entering via the bottom boundary is

$$\frac{dN_2}{dt} = \rho \frac{dp}{dt} dq = \rho \, \dot{p} \, dq \,. \tag{290}$$

To evaluate how the rate at which systems leave the test volume on the right side, one finds the flow by Taylor expansion of the flow density $\rho \dot{q}$ in q up to the first order:

$$\frac{dN_3}{dt} = \left(\rho \,\dot{q} + \frac{\partial}{\partial q} (\rho \,\dot{q}) \,dq + \ldots\right) dp \,. \tag{291}$$

In a similar way, the rate of systems leaving through the top border is

$$\frac{dN_4}{dt} = \left(\rho \,\dot{p} + \frac{\partial}{\partial p} (\rho \,\dot{p}) \,dp + \ldots\right) dq \,. \tag{292}$$

Summing up the net flow of systems into the area dq dp, we get

$$\frac{dN}{dt} = \frac{dN_1}{dt} + \frac{dN_2}{dt} - \frac{dN_3}{dt} - \frac{dN_4}{dt}$$

$$= -\left[\frac{\partial}{\partial q}(\rho \dot{q}) + \frac{\partial}{\partial p}(\rho \dot{p})\right] dq dp$$

$$= -\left[\frac{\partial \rho}{\partial q} \dot{q} + \rho \frac{\partial \dot{q}}{\partial q} + \frac{\partial \rho}{\partial p} \dot{p} + \rho \frac{\partial \dot{p}}{\partial p}\right] dq dp \tag{293}$$

Using the Hamilton equations of motion (278) for the second and last term,

$$\frac{\partial \dot{q}}{\partial q} = \frac{\partial}{\partial q} \left(\frac{\partial H}{\partial p} \right) = \frac{\partial^2 H}{\partial q \partial p} \quad \text{and} \quad \frac{\partial \dot{p}}{\partial p} = \frac{\partial}{\partial p} \left(-\frac{\partial H}{\partial q} \right) = -\frac{\partial^2 H}{\partial q \partial p}, \tag{294}$$

one can see that they vanish, and that

$$\frac{dN}{dt} = -\left[\frac{\partial \rho}{\partial q}\dot{q} + \frac{\partial \rho}{\partial p}\dot{p}\right]dq\,dp\,. \tag{295}$$

Up to here, we have considered only the flux into the area dq dp (or the phase space volume) of a single coordinate/momentum pair (q, p) by balancing the flux through the sides of this volume. For s degrees of freedom (or q_k/p_k pairs), the phase space volume dv is not a square, but a hypercube in 2s dimensions, with 2s surfaces. We can balance the flux into dv in a similar way as for one dimension, but need to replace the width dp of side 1 in expression (289) by the "area" $ds_{1,k}$ of surface (1,k) of the hypercube:

$$dq \, dp \to ds_{1,k} = (dq_1 \, dq_2 \cdots dq_{k-1} \, dq_{k+1} \cdots dq_s)(dp_1 \cdots dp_s).$$
 (296)

With this, the rate of systems entering via surface (1, k) is

$$dN_{1,k} = \rho \,\dot{q}_k \,ds_{1,k} \,dt \,. \tag{297}$$

The difference between the opposing hypersurfaces (1, k) and (3, k) becomes

$$dN_{1,k} - dN_{3,k} = -\frac{\partial}{\partial q_k} (\rho \dot{q}_k) dq_k ds_{1,k} dt$$

$$= -\frac{\partial}{\partial q_k} (\rho \dot{q}_k) dv dt$$

$$= -\left[\frac{\partial \rho}{\partial q_k} \dot{q}_k + \rho \frac{\partial \dot{q}_k}{\partial q_k} \right] dv dt$$
(298)

A similar argument holds for the opposing hypersurfaces (2, k) and (4, k). When summing up the flux through all surfaces, the terms containing $\partial \dot{q}_k/\partial q_k$ and

 $\partial \dot{p}_k/\partial p_k$ vanish again because of (294). This leads to a total number

$$dN = \left(\sum_{k} dN_{1,k} + dN_{2,k} - dN_{3,k} - dN_{4,k}\right) dt$$
$$= -\sum_{k} \left[\frac{\partial \rho}{\partial q_{k}} \dot{q}_{k} + \frac{\partial \rho}{\partial p_{k}} \dot{p}_{k}\right] dv dt \tag{299}$$

of systems entering the phase space volume dv in time dt.

Since the number of systems moving in phase space can not change, the influx dN into dv must cause a change in the phase space density ρ in time:

$$dN = \frac{\partial \rho}{\partial t} \, dv \, dt \,. \tag{300}$$

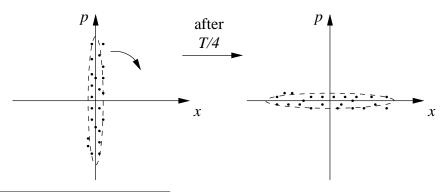
Comparing this with (299) and omitting dv and dt leads to

$$\frac{\partial \rho}{\partial t} = -\sum_{k} \left[\frac{\partial \rho}{\partial q_{k}} \dot{q}_{k} + \frac{\partial \rho}{\partial p_{k}} \dot{p}_{k} \right] , \qquad (301)$$

and after reordering

$$\frac{\partial \rho}{\partial t} + \sum_{k} \left[\frac{\partial \rho}{\partial q_{k}} \dot{q}_{k} + \frac{\partial \rho}{\partial p_{k}} \dot{p}_{k} \right] = \frac{d}{dt} \rho = 0.$$
 (302)

This result is referred as Liouville's theorem¹⁰, and states that the density ρ of points in phase space under time evolution according to Hamilton's equation stays constant. To understand what this result means, we consider an ensemble of systems subject to the motion of a harmonic oscillator, described by the Hamilton function H in (286). The ensemble should be initially distributed over a large range of positions x with a small spread in momentum p and thus little kinetic energy. A quarter of an oscillation period $T = 2\pi/\omega$ later, the distribution has evolved in phase space:



¹⁰published in 1838 by Joseph Liouville, 1809-1882

While the distribution changed its configuration in phase space, the density in the phase space volume that initially contained the distribution did not change, and the large spread in p together with a large spread in x translated to a distribution with a large spread in p and a small spread in p. For the special case of a harmonic oscillator, even the shape of the distribution stays constant, but for more complex systems, the Liouville theorem $d\rho/dt$ still holds, i.e., the *phase space distribution is incompressible* as long as the evolution in time can be described by a Hamilton function, i.e., is non-dissipative.

7.4 Evolution of functions in time and Poisson brackets

Often, one is interested in the time evolution of a quantity that is a function of all coordinates and/or positions of a physical system; the center of mass position in section 4.1, or the total angular momentum in section 4.2 were such examples. In general, such a function can be represented as

$$f = f(\{q_k\}, \{p_k\}, t). \tag{303}$$

Then, the temporal derivative of this function in time can be calculated in the usual way by differentiating with respect to its dependent variables, and using the Hamilton equations of motion (278):

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_{k} \left(\frac{\partial f}{\partial q_{k}} \dot{q}_{k} + \frac{\partial f}{\partial p_{k}} \dot{p}_{k} \right)
= \frac{\partial f}{\partial t} + \sum_{k} \left(\frac{\partial f}{\partial q_{k}} \frac{\partial H}{\partial p_{k}} - \frac{\partial f}{\partial p_{k}} \frac{\partial H}{\partial q_{k}} \right).$$
(304)

By defining the so-called *Poisson bracket* as a short notation,

$$\{f,g\} := \sum_{k} \left(\frac{\partial f}{\partial q_k} \frac{\partial g}{\partial p_k} - \frac{\partial f}{\partial p_k} \frac{\partial g}{\partial q_k} \right),$$
 (305)

the temporal derivative can be written as

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \{f, H\} \tag{306}$$

This is a notation that resembles closely the expression for the time evolution of an operator in a system in quantum physics. Some other properties of these Poisson brackets that are very closely related to corresponding expressions quantum physics can also be verified:

$$\{q_i, p_j\} = \sum_{k} \left(\frac{\partial q_i}{\partial q_k} \frac{\partial p_j}{\partial p_k} - \underbrace{\frac{\partial q_i}{\partial p_k}}_{=0} \underbrace{\frac{\partial p_j}{\partial q_k}}_{=0} \right)$$

$$= \sum_{k} \delta_{ik} \delta_{jk} = \delta_{ij}, \qquad (307)$$

and similarly, for Poisson brackets between coordinates:

$$\{q_i, q_j\} = \sum_{k} \left(\frac{\partial q_i}{\partial q_k} \underbrace{\frac{\partial q_j}{\partial p_k}}_{=0} - \underbrace{\frac{\partial q_i}{\partial p_k}}_{=0} \underbrace{\frac{\partial q_j}{\partial q_k}}_{=0} \right) = 0,$$
 (308)

and with a similar argument, $\{p_i, p_j\} = 0$. In general, two functions f and g are said to *commute with each other* if

$$\{f, g\} = 0. (309)$$

A useful expression can be obtained by evaluating the Poisson bracket with a momentum p_i :

$$\{p_i, f\} = \sum_{k} \left(\underbrace{\frac{\partial p_i}{\partial q_k}}_{=0} \frac{\partial f}{\partial p_k} - \underbrace{\frac{\partial p_i}{\partial p_k}}_{=\delta_{ik}} \frac{\partial f}{\partial q_k} \right)$$

$$= -\sum_{k} \left(\delta_{ik} \frac{\partial f}{\partial q_k} \right) = -\frac{\partial f}{\partial q_i}. \tag{310}$$

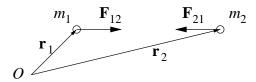
Again, a symmetric expression can be obtained for a Poisson bracket with q_i :

$$\{q_i, f\} = \frac{\partial f}{\partial p_i}. \tag{311}$$

Poisson brackets allow compactly formulating the evolution in time and the relation between different functions of the state of the system characterized by a set of dynamic variables $\{q_k, p_k\}$. They are very closely related to the commutators on quantum physics; in fact, one of the ways to make a transition from classical mechanics to quantum physics simply postulates particular properties of the commutators between operators that differ from classical physics, and take over the rest of the dynamics from the tool set developed in classical Hamiltonian mechanics.

8 Central force motion and two-body problem

One of the both historically and practically important problems in classical mechanics is the dynamics of two objects that exert a central force on each other. As a reminder, central forces were defined as forces that two point masses exert on each other along their distance vector:



Such forces are found in the gravitational interaction between celestial bodies and in the Coulomb interaction between charged particles, and often are in good approximation not subject to dissipation.

8.1 Simplification through conservation laws

Central forces only depend on the difference vector between the positions, and thus can be derived from a potential that only depends on the distance vector:

$$\mathbf{F} = \mathbf{F}(\mathbf{r}_1 - \mathbf{r}_2)$$
 and $U = U(\mathbf{r}_1 - \mathbf{r}_2)$. (312)

Furthermore, since the form of the potential does not depend on the orientation of the distance vector $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ between the two masses, the potential is only a function of the distance $r = |\mathbf{r}|$, so $U = U(|\mathbf{r}|) = U(r)$. The Lagrange function of the system is given by

$$L = \frac{1}{2}m_1\dot{\mathbf{r}}_1^2 + \frac{1}{2}m_2\dot{\mathbf{r}}_2^2 + U(r).$$
(313)

As we have seen in section 4.1, a system of particles with central forces between the particles without external forces has a constant total momentum, and the motion of the center-of-mass position

$$\mathbf{R} = \frac{1}{m_1 + m_2} (m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2) \tag{314}$$

is uniform, i.e., $\ddot{\mathbf{R}}=0$. Therefore, we can choose an inertial system where $\dot{\mathbf{R}}=0$. Next, we place the coordinate origin into the center-of-mass position, so $\mathbf{R}=0$. We then we express the positions $\mathbf{r}_1, \mathbf{r}_2$ via the distance vector \mathbf{r} :

$$\mathbf{r}_1 = \frac{m_2}{m_1 + m_2} \mathbf{r} \quad \text{and} \quad \mathbf{r}_2 = -\frac{m_1}{m_1 + m_2} \mathbf{r} \,.$$
 (315)

With this, the Lagrange function of the problem becomes

$$L = \frac{1}{2}\mu\dot{\mathbf{r}}^2 + U(|\mathbf{r}|) \quad \text{with} \quad \mu := \frac{m_1 m_2}{m_1 + m_2}.$$
 (316)

The quantity μ is referred to as the *reduced mass* of the two-body problem. With this, the original two-body problem has been reduced to a single body problem, with only the distance vector \mathbf{r} as a dynamic variable.

The Lagrange function does not depend on the orientation of \mathbf{r} , only its modulus $|\mathbf{r}|$ via $U(|\mathbf{r}|) = U(r)$. This means that the problem is spherically symmetric, so the Noether theorem in 6.3.2 implies that the angular momentum

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \tag{317}$$

is constant in time. By definition, vectors \mathbf{r} and \mathbf{p} are perpendicular to \mathbf{L} , so they stay in a fixed plane perpendicular to the constant \mathbf{L} . This reduces the problem to a two-dimensional problem in this plane. An adequate set of coordinates are polar coordinates (r, θ) with

$$\mathbf{r} = r \begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix}$$
 and $\dot{\mathbf{r}} = \dot{r} \begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix} + r \begin{pmatrix} -\sin \theta \\ \cos \theta \end{pmatrix} \dot{\theta}$ (318)

in the plane perpendicular to L. With this, $\dot{\mathbf{r}}^2$ in (316) becomes

$$\dot{\mathbf{r}}^2 = \dot{r}^2 + r^2 \dot{\theta}^2 \,, \tag{319}$$

and the Lagrange function simplifies to

$$L = \frac{1}{2}\mu(\dot{r}^2 + r^2\dot{\theta}^2) - U(r) = L(r, \dot{r}, \dot{\theta}).$$
 (320)

As θ is a cyclic coordinate, the corresponding Lagrange equation (206) for θ states just that the corresponding angular momentum

$$p_{\theta} = \frac{\partial L}{\partial \theta} = \mu r^2 \dot{\theta} = const. =: l$$
 (321)

is a constant of motion or a *first integral*. This constant angular momentum $l = |\mathbf{L}|$ has a simple geometric interpretation. The area dA that the radius vector \mathbf{r} covers in a time interval dt can be calculated via

$$rd\theta \qquad dA = \frac{1}{2}r(rd\theta) = \frac{1}{2}r^2d\theta, \qquad (322)$$

so the change of this are in time is given by

$$\frac{dA}{dt} = \frac{1}{2}r^2\dot{\theta} = \frac{l}{2\mu} = const. \tag{323}$$

This is referred to as Kepler's second law^{11} , which at that time was a heuristic description of the positions of the planet Mars recorded by T. Brahe¹². While

¹¹published in 1609 by Johannes Kepler, 1571-1630

¹²Tycho Brahe, 1546-1601

first found with the gravitational interaction, this law holds for any form of the potential U(r) in a central force problem, as it is only a consequence of angular momentum conservation.

The remaining equation of motion is for the distance r between the two bodies,

$$\frac{\partial L}{\partial r} - \frac{d}{dt} \frac{\partial L}{\partial \dot{r}} = \mu r \dot{\theta}^2 - \frac{\partial U}{\partial r} - \frac{d}{dt} (\mu \dot{r})$$

$$= \frac{l^2}{\mu r^3} - \frac{\partial U}{\partial r} - \mu \ddot{r} = 0$$
(324)

or

$$\ddot{r} - \frac{l^2}{\mu^2 r^3} + \frac{1}{\mu} \frac{\partial U}{\partial r} = 0. \tag{325}$$

This is an ordinary differential equation in r that does not have a simple analytical solution for a general potential U(r). However, a number of qualitative observations can be made by looking at the total energy E of the system (which is conserved, as L is independent of t):

$$E = T + U = \frac{1}{2}\mu\dot{r}^2 + \frac{l^2}{2\mu r^2} + U(r).$$
 (326)

This expression can be resolved for the radial velocity \dot{r} ,

$$\dot{r} = \frac{dr}{dt} = \pm \sqrt{\frac{2}{\mu} \left(E - U(r) - \frac{l^2}{2\mu r^2} \right)}.$$
 (327)

Collecting all terms that depend on r on one side and subsequent direct integration leads to

$$t = \int_{r_0}^{r} \frac{dr'}{\sqrt{\frac{2}{\mu} \left(E - U(r') - \frac{l^2}{2\mu r'^2} \right)}} = t(r, r_0), \qquad (328)$$

where r_0 is the distance at t = 0. If the integral can be carried out explicitly, The result can be inverted for the solution $r(t, r_0)$.

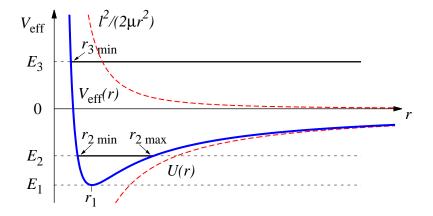
8.2 Effective potential in central force motion

Before moving on to a solution of the radial motion, it is helpful to group the expression (326) into a part dependent on the radial velocity \dot{r} , and the rest:

$$E = \frac{1}{2}\mu\dot{r}^2 + \underbrace{\frac{l^2}{2\mu r^2} + U(r)}_{=:V_{\text{eff}}(r)}.$$
 (329)

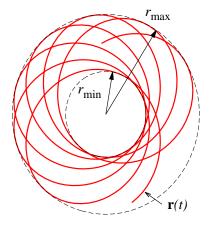
The so-called effective Potential $V_{\text{eff}}(r)$ captures both the original potential U(r), and the kinetic energy $l^2/2\mu r^2$ associated with the angular momentum (sometimes referred to as centrifugal energy), which diverges to positive values for

 $r \to 0$. In a similar way that comparing of the potential with the total energy in (3.3.1) allowed a classification of solutions, one can use the effective potential to make statements on the radial motion of the system. We consider the case of an attractive potential U(r) = -k/r with some l > 0:



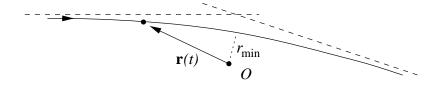
For $E=E_1$, the system is in a state where all the energy is taken up by the effective potential energy, and nothing is left for any radial motion. Therefore, $\dot{r}=0$, so r is constant in time. This does not mean that there is no kinetic energy – there is still the motion connected with the angular momentum l as part of the effective potential $V_{\rm eff}$. The fixed r implies a circular trajectory (with radius r_1), i.e., the system is in a bound state.

For $E = E_2$, the system is also in a bound state, but there is enough energy to allow for radial motion, oscillating between two extremal radii $r_{2\text{min}}$ and $r_{2\text{max}}$ with an oscillation period that can be calculated via (328). The trajectory or orbit $\mathbf{r}(t)$ could look like this:



The motion in radial direction and the one due to the angular momentum l are not necessarily synchronized for all potentials U(r) – in the figure above, they are not. In this case the orbit is referred to as *open*.

For $E=E_3$, there is only one intersection of $V_{\rm eff}(r)$ with the line of constant energy at $r_{\rm 3min}$, which means that the particle moves from infinity to the point of closest proximity to the origin (corresponding to the center of mass of the system), and then leaves again with $r(t \to +\infty) \to \infty$. Because $U(r \to \infty) \to 0$, the particle approaches the center from an asymptotically uniform motion, interacts with the other particle and then escapes, approaching a uniform motion into a different direction:



This situation is referred to as a *scattering process*, and is an important concept in atomic, molecular and particle physics.

We now come back to the problem of solving the radial motion in (325). To assess the shape of orbits without considering the explicit time dependency, we convert (325) into an equation for $r(\theta)$. For this, we introduce the substitution

$$u := \frac{1}{r} \tag{330}$$

and calculate its derivatives with respect to θ (using $l = \mu r^2 \dot{\theta}$):

$$\frac{du}{d\theta} = -\frac{1}{r^2}\frac{dr}{d\theta} = -\frac{1}{r^2}\frac{dr}{dt}\frac{dt}{d\theta} = -\frac{1}{r^2}\dot{r}\frac{1}{\dot{\theta}} = -\dot{r}\frac{\mu}{l},\tag{331}$$

and

$$\frac{d^2u}{d\theta^2} = -\frac{\mu}{l}\frac{d\dot{r}}{d\theta} = -\frac{\mu}{l}\frac{d\dot{r}}{dt}\frac{dt}{d\theta} = -\frac{\mu}{l}\frac{1}{\dot{\theta}}\ddot{r} = -\frac{\mu^2}{l^2}r^2\ddot{r}.$$
 (332)

This can be used to substitute \ddot{r} in (325) by

$$\ddot{r} = \frac{d^2u}{d\theta^2} \left(-\frac{l^2}{\mu^2 r^2} \right), \tag{333}$$

so the differential equation (325) becomes

$$-\frac{l^2}{\mu r^2} \frac{d^2 u}{d\theta^2} - \frac{l^2}{\mu r^4} r = -\frac{\partial U}{\partial r} \quad \text{or}$$

$$\frac{d^2 u}{d\theta^2} + u = \frac{\mu}{l^2} r^2 \frac{\partial U}{\partial r}$$
(334)

This is a simpler differential equation that can be solved for the important class of potentials where $U \propto 1/r$.

8.3 Kepler problems

Two-body problems with a potential

$$U = -\frac{k}{r} \tag{335}$$

are referred to as *Kepler problems*, because they are equivalent to solving the planetary motion problem. For gravitational attraction,

$$k = Gm_1m_2, (336)$$

with the gravitational constant G and the heavy masses m_1 and m_2 . For the coulomb interaction,

$$k = -\frac{q_1 q_2}{4\pi\epsilon_0} \,, (337)$$

for two charges q_1, q_2 , with the electrical permittivity ϵ_0 . The minus sign takes into account that charges of the same sign repel each other, while charges of opposite sign attract each other. The potential (335) leads to a radial derivative $\partial U/\partial r \propto r^{-2}$, which simplifies the differential equation (334) to

$$\frac{d^2u}{d\theta^2} + u - c = 0 \quad \text{with} \quad c = \frac{\mu}{l^2} k = const. \tag{338}$$

This is a simple linear differential equation with special solutions of the form

$$u(\theta) = Ae^{B\theta} + c, (339)$$

with the same c as in (338). Inserting this solution into (338) leads to $B^2 = -1$, or a general solution

$$u(\theta) = A'e^{i\theta} + A''e^{-i\theta} + c, \qquad \text{or} \quad u(\theta) = A'''\cos(\theta - \theta_0) + c. \tag{340}$$

with free integration constants A' and A'', or A''' and θ_0 that are suitable for a description of the real-valued solution. We can choose $\theta_0 = 0$, because this only orients our polar coordinate system in a particular way. The integration constant A''' needs then to be determined form the initial conditions. Re-arranging the solution into a different form yields

$$\frac{u}{c} = \frac{1}{c} \frac{1}{r} = \frac{A'''}{c} \cos \theta + 1.$$
 (341)

With a transition to the the common definitions

$$\alpha := \frac{1}{c} = \frac{l^2}{\mu k}$$
 and $\epsilon := \frac{A'''}{c}$, (342)

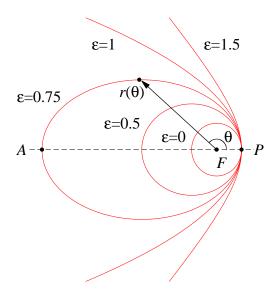
the solution takes the form

$$\frac{\alpha}{r} = 1 + \epsilon \cos \theta \,. \tag{343}$$

This is the parametric description of a number of curves referred to as *cone* intersections, and the dimensionless constant ϵ in this expression is referred to as the eccentricity of the curve.

8.3.1 Classification of orbits

The cone intersections as solutions for the Kepler problem can be classified according to the values of the eccentricity ϵ ; in the graph below, α was chosen such that all trajectories have the same distance of the nearest point P on the trajectory to the origin F:



- For $\epsilon = 0$, the solution for $r(\theta) = \alpha$ is independent of θ , and the trajectory is a circle around the coordinate origin. This corresponds to the bound state with the lowest total energy for a given angular momentum l.
- For 0 < ε < 1, the trajectory r(θ) forms an ellipse, with the coordinate origin in one of its focal points F. The trajectory represents again a bound state. Point P on the trajectory is the one with the closest distance to the coordinate origin, and therfore the shortest distance between the two bodies. It is referred to as pericenter, or, if reference is made to a planet orbiting the Sun, as perihelion, or as perigee if reference is made to a satellite orbiting the earth. Similarly, the position A on the trajectory which is furthest away from the coordinate origin is referred to as apocenter, apohelion, or apogee, respectively. If one of the two masses is much heavier than the other one, its distance from the center of mass of the system (i.e the coordinate origin) is very small, and therefore would be located near the focal point F of the elliptical orbit. This is Kepler's first law for planetary motion, stating that planetary orbits are ellipses, with the Sun in one of its foci.</p>

- For $\epsilon = 1$, the solution $r(\theta)$ represents a parabola. This corresponds to the situation where E = 0. It is not a bound state anymore, because $r(t \to \pm \infty) \to \infty$.
- For $\epsilon > 1$, the trajectories are also not bounded. Furthermore, the range of θ is limited because expression (343) diverges for $\theta \to \theta_{\text{max}}$, with

$$\cos \theta_{\text{max}} = -\frac{1}{\epsilon} \,. \tag{344}$$

In this case, the trajectory starts out with $\theta = \theta_{\text{max}}$ and $r \to \infty$, moves towards the coordinate center, with a decreasing θ , reaches the pericenter P for $\theta = 0$, and leaves for $r \to \infty$ with $\theta \to -\theta_{\text{max}}$ (or the other way round). Such a problem is referred to as a scattering problem.

So far, we have discussed the solutions (343) to the Kepler problem only qualitatively. We still need to make the connection of the orbit parameter ϵ with the physical properties of the two body problem, since α is already fixed via (342).

The connection is easily made by using expression (326) for the total energy, and inserting the Kepler potential:

$$E = T + U = \frac{1}{2}\mu\dot{r}^2 + \frac{1}{2}\frac{l^2}{\mu r^2} - \frac{k}{r}$$
 (345)

By definition, the radial velocity \dot{r} a the pericenter $r = r_{\min}$ vanishes

$$E = \frac{1}{2} \frac{l^2}{\mu r_{\min}^2} - \frac{k}{r_{\min}} \tag{346}$$

On the other hand, we have an expression for r_{\min} from the Kepler solution (343):

$$r_{\min} = \frac{\alpha}{1+\epsilon} \,. \tag{347}$$

Inserting this into the expression for the total energy (346) yields

$$E = \frac{1}{2} \frac{l^2}{\mu} \frac{(1+\epsilon)^2}{\alpha^2} - k \frac{1+\epsilon}{\alpha}$$
$$= \frac{k}{\alpha} \left[\frac{1}{2} (1+\epsilon)^2 - (1+\epsilon) \right] = \frac{k}{2\alpha} \left[\epsilon^2 - 1 \right]. \tag{348}$$

This expression can be inverted into

$$\epsilon = \sqrt{\frac{2\alpha E}{k} + 1} = \sqrt{1 + E\frac{2l^2}{\mu k^2}}.$$
(349)

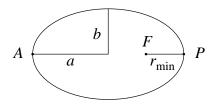
With this, the orbit parameters α , ϵ are fully determined by the orbital momentum l and the total energy E of the two-body problem. Alternatively, a particular

velocity at a position in space could have been specified as an initial condition, but l and E can always easily be calculated from them.

As a last step in this section, we want to apply Kepler's second law (323), and evaluate the total orbital period τ of a bound state by equating the area covered by the radius vector per unit of time with the ratio of the ellipse area A and τ :

$$\frac{dA}{dt} = \frac{l}{2\mu} \stackrel{!}{=} \frac{A}{\tau} = \frac{\pi ab}{\tau},\tag{350}$$

where a and b are the two semi-axes of an elliptical or circular orbit.



One can easily show that a and b are connected with the parameters ϵ and α of the cone intersection expression (343):

$$a = \frac{\alpha}{1 - \epsilon^2}$$
 and $b = \sqrt{\alpha a}$. (351)

With this, one finds with $l = \sqrt{\alpha \mu k}$ from (342)

$$\tau = \pi a b \frac{2\mu}{l} = \pi a^{3/2} \sqrt{\alpha} \frac{2\mu}{\sqrt{\alpha \mu k}} = a^{3/2} \pi \sqrt{\frac{4\mu}{k}}.$$
 (352)

This leads to

$$\frac{\tau^2}{a^3} = \frac{4\pi^2 \mu}{k} = const., (353)$$

which to a good approximation is Kepler's third law, stating that the ratio of τ^2 and the cube of the semi-major axis a of a planetary orbit is a constant for all planets orbiting around the sun. The latter can be seen by recalling the expressions for the reduced mass μ from (316) and $k = Gm_1m_2$ for a gravitational potential:

$$\frac{4\pi^2\mu}{k} = 4\pi^2 \frac{m_1 m_2}{m_1 + m_2} \frac{1}{Gm_1 m_2} = \frac{4\pi^2}{G(m_1 + m_2)} \approx \frac{4\pi^2}{Gm_2},$$
 (354)

since the mass m_2 of the Sun is much larger the mass m_1 of any planet.

8.3.2 Orientation of elliptical orbits: Laplace-Runge-Lentz vector

In the previous section, we have seen some aspects of stable orbits for Kepler problems with

$$U(\mathbf{r}) = -\frac{k}{r}$$
 and $\mathbf{F} = -\nabla U = -\frac{k}{r^3}\mathbf{r}$. (355)

One of the consequences of the conservation of angular momentum **L** was that the motion takes place in a plane only. Implicit in the solutions for the elliptical orbits was that the semi-major axis is a constant in time, i.e., its orientation in space is fixed. When determining the integration constants in (340), we chose $\theta_0 = 0$, and aligned the coordinate system with the semi-major axis.

In practice, the orientation of the semi-major axis (and even the whole equations of motion) can be obtained from a specific vector. We define

$$\mathbf{A} := \mathbf{p} \times \mathbf{L} - \mu k \frac{1}{r} \mathbf{r} \,, \tag{356}$$

with the momentum \mathbf{p} , angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ and position vector \mathbf{r} . This quantity is referred to as *Laplace-Runge-Lentz vector*, or sometimes only as Runge-Lentz vector. It lies in the plane of motion (because the first component of (356) is perpendicular to \mathbf{L} , and the second component is in the plane of motion anyways). To show that this vector is a constant of motion, we calculate at the temporal derivative of its first component:

$$\frac{d}{dt}(\mathbf{p} \times \mathbf{L}) = \dot{\mathbf{p}} \times \mathbf{L} + \mathbf{p} \times \underbrace{\dot{\mathbf{L}}}_{=0}$$
(357)

Using $\dot{\mathbf{p}} = \mathbf{F} = -k\mu \mathbf{r}/r^3$ and $\mathbf{p} = \mu \dot{\mathbf{r}}$, we can continue

$$\frac{d}{dt}(\mathbf{p} \times \mathbf{L}) = -\frac{k\mu}{r^3} (\mathbf{r} \times (\mathbf{r} \times \dot{\mathbf{r}}))$$

$$= -\frac{k\mu}{r^3} ((\mathbf{r} \cdot \dot{\mathbf{r}})\mathbf{r} - (\mathbf{r} \cdot \mathbf{r})\dot{\mathbf{r}})$$

$$= -\frac{k\mu}{r^3} (r\dot{r}\,\mathbf{r} - r^2\,\dot{\mathbf{r}})$$

$$= k\mu \left(-\frac{1}{r^2}\dot{r}\,\mathbf{r} + \frac{1}{r}\dot{\mathbf{r}} \right) = k\mu \frac{d}{dt} \left(\frac{1}{r}\mathbf{r} \right) . \tag{358}$$

The step from the second to thrid line can be seen by writing $\mathbf{r} = r \, \mathbf{e}_r$, differentiating this product with respect to time to get $\dot{\mathbf{e}}_r$, and using $\mathbf{e}_r \perp \dot{\mathbf{e}}_r$. Then, the expression can be re-arranged into

$$\frac{d}{dt}\left(\mathbf{p} \times \mathbf{L} - k\mu \frac{1}{r}\mathbf{r}\right) = \frac{d}{dt}\mathbf{A} = 0.$$
(359)

Thus, the Laplace-Runge-Lentz vector is conserved over time. Its orientation with respect to the elliptical motion can be seen by forming the scalar product

with the position vector \mathbf{r} :

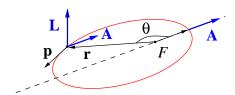
$$\mathbf{A} \cdot \mathbf{r} = \mathbf{r} \cdot (\mathbf{p} \times \mathbf{L}) - \mu k \frac{\mathbf{r} \cdot \mathbf{r}}{r}$$

$$= \mathbf{L} \cdot \underbrace{(\mathbf{r} \times \mathbf{p})}_{=\mathbf{L}} - \mu k r = l^2 - \mu k r.$$
(360)

On the other side, $\mathbf{A} \cdot \mathbf{r} = A r \cos \theta$, where $A = |\mathbf{A}|$ and θ is the angle between vectors \mathbf{A} and \mathbf{r} . Reordering this expression into

$$\frac{l^2}{\mu k r} = 1 + \frac{A}{\mu k} \cos \theta \tag{361}$$

suggests that the angle θ here is the same as in the solutions for the cone intersections in (343). Thus, for $\theta = 0$, the vector **A** points in the same direction as **r**, namely in the direction of the pericenter, parallel to the semi-major axis of the ellipse:

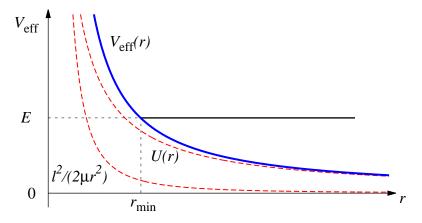


Direct comparison of (361) with the expression for the cone intersections (343) also reveals the connection between the length of the Laplace-Runge-Lentz vector and the eccentricity:

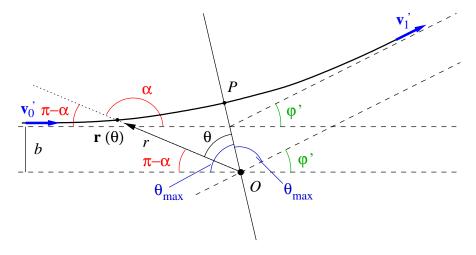
$$A = \mu k \epsilon \tag{362}$$

8.4 Scattering orbits

We now come back to the orbits in section (8.2) corresponding to a total energy E > 0, such that $\mathbf{r}(t)$ is not bounded, i.e., $r(t \to \pm \infty) \to \infty$. This is also the only type of solutions for potentials modeling the two-body interaction that are repulsive:



Typically, the interactions U(r) vanish for large r; there, the particle is in uniform motion with a constant velocity $\dot{\mathbf{r}} = \mathbf{v}_0'$. The prime with the velocity should indicate that reference is made to a relative velocity between the two bodies, because we still are in the framework of an effective one-body problem. The vector \mathbf{r} will move towards the pericenter P with a minimal distance from the center-of-mass position (or coordinate origin O), and then move away again. For $r \to \infty$, the motion becomes uniform again, with a new constant velocity \mathbf{v}_1' . As we are still looking at a conservative interaction, the velocities have the same modulus, but a different direction. Asymptotically, the effect of the two-body interaction is a deflection of the particle by an angle φ' . The geometry of that interaction is shown in the diagram below:



First, we note that the scattering angle φ' between the asymptotic velocities \mathbf{v}_0'

and \mathbf{v}'_1 is determined by the maximal angle θ_{max} in the polar coordinate system (oriented in the direction O-P in the figure):

$$\varphi' = \pi - 2\theta_{\text{max}} \tag{363}$$

For any two-body central force problem, the angular momentum is a conserved quantity. We therefore try to evaluate it from the geometric parameters shown in the above diagram, using

$$l = |\mathbf{L}| = |\mathbf{r} \times \mathbf{p}| = \mu |\mathbf{r} \times \mathbf{v}_0'| = \mu r v_0' \sin \alpha = \mu r v_0' \sin(\pi - \alpha), \qquad (364)$$

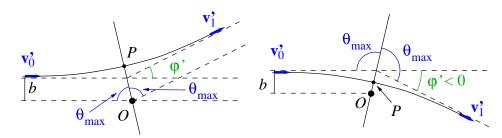
where here, α is the angle between \mathbf{r} and \mathbf{v}'_0 . Asymptotically, the expression

$$r\sin(\pi - \alpha) =: b \tag{365}$$

measures the shortest distance b between the trajectory the particle would have taken without interaction, and the coordinate origin. The distance b is referred to as *impact parameter* of the scattering trajectory, and measures, casually speaking, how far the scattering center O was missed if there were no interaction. With this, one can fix the angular momentum to

$$l = \mu v_0' b \tag{366}$$

The diagram above shows a scattering problem for a repulsive potential. By convention, the scattering angle φ' in this case is counted positively. For a scattering problem with an attractive potential the scattering angle is negative, compatible with definition (363):



Since the scattering angle φ' is a simple function (363) of the maximum angle θ_{max} of the trajectory in a polar coordinate system with the $\theta=0$ direction defined by the direction O-P, we try to evaluate this angle for a general potential U(r). For this, we go back to the expression (327) for the radial velocity in a central force problem:

$$\dot{r} = \frac{dr}{dt} = \pm \sqrt{\frac{2}{\mu} \left(E - U(r) - \frac{l^2}{2\mu r^2} \right)}.$$
 (367)

We are interested in an expression $\theta(r)$, so we use the above expression to construct a useful derivative:

$$\frac{d\theta}{dr} = \frac{d\theta}{dt} \frac{dt}{dr} = \frac{\dot{\theta}}{\dot{r}}$$

$$= \frac{l}{\mu r^2} \frac{1}{\dot{r}} = \frac{l}{\mu r^2} \frac{1}{\pm \sqrt{\cdots}}.$$
(368)

Sorting again components that depend on r on one side leads to

$$d\theta = \frac{l}{\mu r^2} \frac{dr}{\pm \sqrt{\cdots}},\tag{369}$$

which we integrate from the pericenter (at $\theta = 0$) to infinity. Since the distance r increases monotonously, we can choose the positive sign (assuming l > 0), and get an expression for θ_{max} :

$$\theta_{\text{max}} = \int_{r_{\text{min}}}^{+\infty} \frac{l \, dr}{\mu r^2 \sqrt{\frac{2}{\mu} \left(E - U(r) - \frac{l^2}{2\mu r^2} \right)}} \,. \tag{370}$$

To carry out this integration, we still need to know the r_{\min} , which can be obtained from (327), knowing that at r_{\min} , the radial velocity \dot{r} vanishes:

$$E - U(r_{\min}) - \frac{l}{2\mu r_{\min}^2} = 0.$$
 (371)

This equation needs to be solved for the integration boundary r_{\min} in (370), leading to the maximal polar angle $\theta_{\max} = \theta_{\max}(E, l)$. The energy E in the system is the energy in the center-of-mass system, so we should note it as

$$E' = \frac{\mu v_0'^2}{2} \,. \tag{372}$$

As the angular momentum in a scattering problem is conveniently given by the impact parameter b via (366), the scattering angle φ' becomes only a function of b and v'_0 , or b and E'.

8.4.1 Scattering angle for Kepler problems

For general potentials U(r), it can be difficult or impossible to obtain the maximal polar angle θ_{max} from (370) in a closed form. For the important Kepler problems introduced in section 8.3 it is possible, but it is even easier to use the result (344):

$$\cos \theta_{\text{max}} = -\frac{1}{\epsilon} \,, \tag{373}$$

with the eccentricity ϵ given by (349). In the parametric equation (343) for the Kepler orbits, we implicitly used k > 0 corresponding to attractive interactions to obtain a radial distance r > 0. However, the sign of the integration constant α in (342) can be changed for k < 0 without affecting any of the derivations, resulting in r > 0 for repulsive interactions, e.g. of two electric charges of the same sign. Expression (349) for ϵ is not affected by this sign change, so θ_{max} can be obtained via (373), resulting in an expression for the scattering angle φ' :

$$-\frac{1}{\epsilon} = \cos \theta_{\text{max}} = \cos \left(\frac{\pi}{2} - \frac{\varphi'}{2}\right) = \sin \frac{\varphi'}{2}. \tag{374}$$

Using (349) for the eccentricity ϵ leads to

$$\sin \frac{\varphi'}{2} = -\frac{1}{\epsilon} = -\left[1 + E' \frac{2l^2}{\mu k^2}\right]^{-1/2}$$

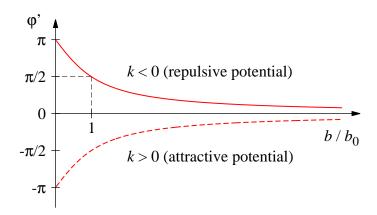
$$= -\left[1 + E' \frac{2\mu^2 v_0'^2 b^2}{\mu k^2}\right]^{-1/2} = -\left[1 + 4E'^2 \frac{b^2}{k^2}\right]^{-1/2}$$

$$= -\left[1 + \frac{b^2}{b_0^2}\right]^{-1/2} \quad \text{with} \quad b_0 := \frac{k}{2E'}. \tag{375}$$

This can be further simplified into

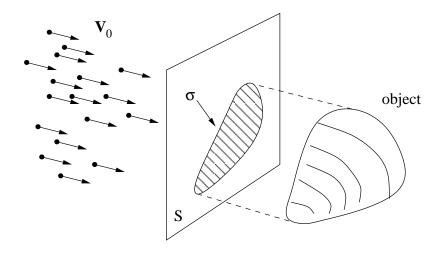
$$\tan\frac{\varphi'}{2} = -\frac{b_0}{b}\,,\tag{376}$$

correctly reflecting the sign convention. The scattering angle φ' is therefore a simple function of the normalized impact parameter b/b_0 , where b_0 has the dimension of a length:



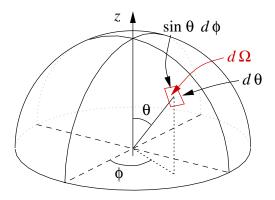
8.5 Scattering cross section

Scattering problems are often described in terms of a scattering cross section. The scattering cross section σ is the effective area an object exposes to projectiles targeting the object from a particular direction. In the simplest form, σ is just the projection of the object onto a screen S perpendicular to the velocity vector \mathbf{v} of the projectiles before the impact:



If the density of the projectiles per screen area is constant, the number of projectiles hitting the object is proportional to its scattering cross section σ .

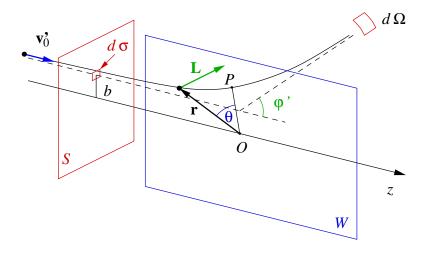
In the previous section, we found a relation between the impact parameter b and the deflection angle φ' for scattering trajectories of two particles that interact via a potential U(r). To connect these trajectories with the concept of a scattering cross section, we first quantify the direction in which projectiles are scattered. A single direction in the 3-dimensional space can be described by two angles θ, ϕ in a spherical coordinate system. The solid angle Ω captures a set of directions in space, and is just the surface area on a unit sphere corresponding to this set of directions. Since the surface of a sphere is $4\pi r^2$, the full solid angle corresponding to all possible directions is $\Omega = 4\pi$, a half space corresponds to $\Omega = 2\pi$. The solid angle is dimensionless, but occasionally, the unit sr (for steradian) is used to indicate that reference is made to a solid angle.



In spherical coordinates, a small set of directions is given by the solid angle element

$$d\Omega = \sin\theta \, d\phi \, d\theta \,. \tag{377}$$

Coming back to scattering orbits in two-body interactions, we need to consider two different coordinate systems. One is the coordinate system in which we describe the two-body interaction. As we have seen in section 8.1, the two-body interaction is a problem in a plane W, characterized by polar coordinates θ, r in the figure below:



Remember that this is an effective one-body problem, assuming a description in an inertial reference frame, with the coordinate origin O centered in the center-of-mass motion of the two-body problem. The angular momentum \mathbf{L} is constant in time, and perpendicular to the plane W of orbital motion.

The other coordinate system is used to describe the deflection of the particle in a coordinate system suitable to describe directions. This is a spherical coordinate system, with the main axis pointing in the direction of the velocity \mathbf{v}'_0 of the effective single body scattered from the origin O. This is a spherical coordinate system, where z axis is aligned parallel to the initial velocity \mathbf{v}'_0 of the projectile.

We consider the surface element $d\sigma$ in the screen plane S that corresponds to a deflection into the direction element $d\Omega$. The ratio

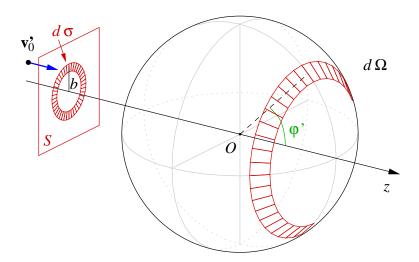
$$\frac{d\sigma}{d\Omega} \tag{378}$$

is referred to as the differential cross section. To calculate this quantity, we first note that the scattering problem for central force interactions is rotationally symmetric around the z axis. Projectiles hitting in a ring of radius b and thickness db with an area

$$d\sigma = 2\pi b \, db \tag{379}$$

will have the same differential cross section, and end up in a ring-shaped set of directions as shown in the figure below, covering a solid angle of

$$d\Omega = 2\pi \sin \varphi' \, d\varphi' \,. \tag{380}$$



With this, we find for the differential scattering cross section

$$\frac{d\sigma}{d\Omega} = \frac{2\pi b \, db}{2\pi \sin \varphi' \, d\varphi'} = \frac{b}{\sin \varphi'} \left| \frac{db}{d\varphi'} \right| \,. \tag{381}$$

The modulus of the derivative $db/d\varphi'$ was taken because for scattering problems with a repulsive potential, $db/d\varphi'$ is negative; the differential cross section is only meaningful for positive values.

8.5.1 Rutherford scattering

An important problem that helped to discover the structure of atoms was the elastic scattering of α particles (positively charged helium nuclei) by the also positively charged nuclei of heavy atoms. To treat this in the framework of classical mechanics, we recall the expression (375) for the deflection angle φ' for scattering orbits in Kepler problems in the previous section:

$$\sin\frac{\varphi'}{2} = -\left[1 + \frac{b^2}{b_0^2}\right]^{-1/2} \tag{382}$$

By squaring and inverting this expression, we get

$$\left(\sin\frac{\varphi'}{2}\right)^{-2} = 1 + \frac{b^2}{b_0^2}\,,\tag{383}$$

which can be differentiated on both sides,

$$-2\sin^{-3}\frac{\varphi'}{2}\cos\frac{\varphi'}{2}\frac{1}{2}\,d\varphi' = \frac{2\,b}{b_0^2}\,db\,, (384)$$

or

$$\frac{db}{d\varphi'} = -\frac{b_0^2 \cos(\varphi'/2)}{\sin^3(\varphi'/2)} \frac{1}{2b},\tag{385}$$

which is negative for all scattering angles $0 \le \varphi' \le \pi$. We use this result in expression (381) for the differential scattering cross section, and obtain

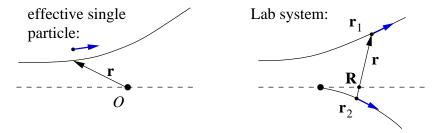
$$\frac{d\sigma}{d\Omega} = \frac{b_0^2 \cos(\varphi'/2)}{2 \sin \varphi' \sin^3(\varphi'/2)}
= \frac{b_0^2}{4 \sin^4(\varphi'/2)} = \frac{k^2}{16E'^2 \sin^4(\varphi'/2)}.$$
(386)

This is a historically and practically important formula for *Rutherford scattering*. The fortunate fact that this result, obtained by classical mechanics, is the same as the one obtained from a quantum mechanical description led to a rapid development of the understanding of the structure of atoms by Rutherford¹³ and coworkers.

8.6 Scattering problems in the laboratory system

The differential scattering cross section $d\sigma/d\Omega$ is very useful because it is directly related to typical scattering experiments. Usually, a scattering target is located somewhere in space, and exposed to a homogenous flux of projectile particles (e.g. Helium nuclei or protons). A typical sample consists of many target particles, and is much larger than a characteristic impact parameter for an individual scattering process, like b_0 in (375). A detector with a fixed size measures the flux of scattered particles at different deflection angles in a fixed distance from the target, so the solid angle subtended by the detector from the view of the scattering target is fixed. The differential scattering cross section is than simply proportional to the detected number of scattered particles in a particular direction.

To make a connection between the differential scattering cross section seen in the lab with the one calculated for the effective one-body problem, we need to find an adequate transformation – first into the centre-of-mass (CM) system, then into the lab.



The center-of-mass position \mathbf{R} of two masses m_1, m_2 at positions \mathbf{r}_1 and \mathbf{r}_2 (in the lab system) was was defined in section 4.1 as

$$\mathbf{R} = \frac{1}{m_1 + m_2} (m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2) = \frac{\mu}{m_2} \mathbf{r}_1 + \frac{\mu}{m_1} \mathbf{r}_2,$$
 (387)

¹³published in Philosophical Magazine **21**, 669-688 (1911) by Ernest Rutherford, 1871-1937

with the effective mass $\mu = m_1 m_2/(m_1 + m_2)$. The coordinate origin in a CM system is chosen such that $\mathbf{R} = 0$. Then, the positions \mathbf{r}'_1 and \mathbf{r}'_2 of both masses in the CM system are connected by

$$m_1 \mathbf{r}'_1 + m_2 \mathbf{r}'_2 = 0, \quad \text{or} \quad \mathbf{r}'_1 = \frac{\mu}{m_1} \mathbf{r}, \quad \mathbf{r}'_2 = -\frac{\mu}{m_2} \mathbf{r}$$
 (388)

with the difference vector

$$\mathbf{r} = \mathbf{r}_1' - \mathbf{r}_2' = \mathbf{r}_1 - \mathbf{r}_2, \tag{389}$$

describing completely the state of the system in the effective single-particle description. With (387) and (389), the positions of particles 1 and 2 in the lab system can be expressed by ${\bf R}$ and ${\bf r}$ according to

$$\mathbf{r}_1 = \mathbf{R} + \mathbf{r}_1' = \mathbf{R} + \frac{\mu}{m_1} \mathbf{r}, \quad \text{and} \quad \mathbf{r}_2 = \mathbf{R} - \frac{\mu}{m_2} \mathbf{r}.$$
 (390)

Similarly, the velocities in the lab system are given by

$$\dot{\mathbf{r}}_1 = \dot{\mathbf{R}} + \frac{\mu}{m_1} \dot{\mathbf{r}} \quad \text{and} \quad \dot{\mathbf{r}}_2 = \dot{\mathbf{R}} - \frac{\mu}{m_2} \dot{\mathbf{r}}. \tag{391}$$

8.6.1 Transformation of energy between lab and CM system

The total kinetic energy of the two particles in the lab system at any time can be expressed by the CM velocity $\dot{\mathbf{r}}$, and the effective single-particle velocity $\dot{\mathbf{r}}$,

$$T = \frac{1}{2}m_{1}\dot{\mathbf{r}}_{1}^{2} + \frac{1}{2}m_{2}\dot{\mathbf{r}}_{2}^{2} = \frac{1}{2}m_{1}\left(\dot{\mathbf{R}} + \frac{\mu}{m_{1}}\dot{\mathbf{r}}\right)^{2} + \frac{1}{2}m_{1}\left(\dot{\mathbf{R}} - \frac{\mu}{m_{2}}\dot{\mathbf{r}}\right)^{2}$$

$$= \frac{1}{2}(m_{1} + m_{2})\dot{\mathbf{R}}^{2} + \frac{1}{2}\left(\frac{\mu^{2}}{m_{1}} + \frac{\mu^{2}}{m_{2}}\right)\dot{\mathbf{r}}^{2}$$

$$= \frac{1}{2}M\dot{\mathbf{R}}^{2} + \frac{1}{2}\mu\dot{\mathbf{r}}^{2} = \frac{1}{2}M\dot{\mathbf{R}}^{2} + T'$$
(392)

with the total mass $M = m_1 + m_2$, and the kinetic energy T' in the CM system. Long before and long after the impact, all the energy is in the kinetic energy of the particles, so

$$E = T = \frac{1}{2}M\dot{\mathbf{R}}^2 + E',$$
 (393)

where E' is the energy in the CM system available for the scattering process.

In a typical scattering scenario, the target mass m_2 is initially at rest in the lab (i.e., $\dot{\mathbf{r}}_2 = 0$), and the projectile mass m_1 moves towards the target with a velocity \mathbf{v}_0 . By differentiating (387), one finds for the CM velocity

$$\dot{\mathbf{R}} = \frac{\mu}{m_2} \mathbf{v}_0 \,. \tag{394}$$

By using (391), one finds

$$\mathbf{v}_0 = \dot{\mathbf{r}}_1 = \frac{\mu}{m_2} \mathbf{v}_0 + \frac{\mu}{m_1} \dot{\mathbf{r}} \quad \text{or} \quad \mathbf{v}_0 = \dot{\mathbf{r}} = \mathbf{v}_0', \tag{395}$$

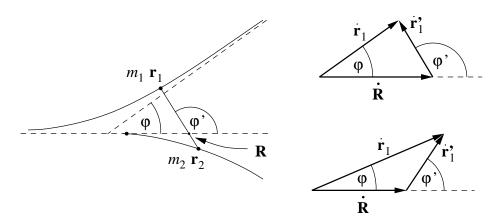
i.e., the velocity \mathbf{v}'_0 in the CM system before the interaction is the same as the initial velocity \mathbf{v}_0 of the projectile in the lab system. Acknowledging that the initial total energy is only given by the kinetic energy $m_1\mathbf{v}_0^2/2$ of the projectile, and using (394) in (393), one finds the simple relation

$$E' = E \frac{m_2}{m_1 + m_2} \tag{396}$$

for the total available energy E' in the CM system, and therefore also in the effective single-particle system. Since the impact parameter b in the lab, the CM system, and in the effective single particle system are the same, we have enough information to calculate the deflection angle $\varphi' = \varphi'(E', b)$ (in the effective single particle systm) from a known energy E in the lab system. Also note that the angle φ' between \mathbf{r} and \mathbf{v}_0 is the same in the effective single particle system and the CM system.

8.6.2 Transformation of deflection angles between lab and CM system

To transform the deflection angle φ' back to the lab system, we consider the geometrical relationship between velocities \mathbf{r}_1 , \mathbf{r}_2 and \mathbf{r} as shown:



On the left side, the relationship between φ and the asymptotic trajectories in the lab, and the deflection angle φ' with respect to the difference vector \mathbf{r} is shown. On the right side, one can see the corresponding geometry of the velocity relation $\dot{\mathbf{r}}_1 = \dot{\mathbf{R}} + \dot{\mathbf{r}}_1'$ between lab and CM system. Splitting this up into Cartesian components leads to

$$\dot{r}_1 \cos \varphi = \dot{r}'_1 \cos \varphi' + \dot{R} \quad \text{and}$$

$$\dot{r}_1 \sin \varphi = \dot{r}'_1 \sin \varphi'. \tag{397}$$

Note that this expression relates asymptotic velocities, so φ and φ' do not change with time anymore. This can be resolved into a relation between φ and φ' ,

$$\tan \varphi = \frac{\sin \varphi}{\cos \varphi} = \frac{\sin \varphi'}{\cos \varphi' + \gamma}, \quad \text{with} \quad \gamma := \frac{\dot{R}}{\dot{r}_1'} = \frac{m_1}{m_1 + m_2} \frac{v_0}{\dot{r}_1'}, \tag{398}$$

which still depends on the final speed \dot{r}_1' of the projectile in the CM system. To eliminate this, we express the total energy E'=T' in the CM system before the impact by the kinetic energies after the impact, and include a possible energy loss H during the scattering process:

$$E' = \frac{1}{2}m_1\dot{r}_1^{\prime 2} + \frac{1}{2}m_2\dot{r}_2^{\prime 2} + H.$$
 (399)

This can e.g. cover a radiation losses due to the acceleration of charges in the scattering process. The kinetic energy of m_2 can also be expressed by \dot{r}'_1 using momentum conservation in the CM system, leading to

$$E' = \frac{1}{2}m_1 \left(\frac{m_1 + m_2}{m_2}\right) \dot{r}_1^{2} + H.$$
 (400)

By expressing E' by E via (396) and dividing by E, one finds

$$\frac{m_2}{m_1 + m_2} = \frac{1}{E} \frac{1}{2} m_1 \left(\frac{m_1 + m_2}{m_2} \right) \dot{r}_1^{2} + \frac{H}{E}$$
 (401)

or

$$1 = \underbrace{\left(\frac{m_1 + m_2}{m_2}\right)^2 \frac{\dot{r}_1'^2}{v_0^2}}_{=\frac{1}{\gamma^2} \frac{m_1^2}{m_2^2}} + \underbrace{\frac{H}{E} \frac{m_1 + m_2}{m_2}}_{(402)}$$

which can finally be resolved into

$$\gamma^2 = \left(\frac{m_1}{m_2}\right)^2 \frac{1}{1 - \frac{H}{E} \left(\frac{m_1 + m_2}{m_2}\right)}.$$
 (403)

For elastic scattering with H=0, one gets the simple relation

$$\gamma = \frac{m_1}{m_2} \tag{404}$$

for use in the transformation (398) between deflection angles φ and φ' .

8.6.3 Transformation of the differential scattering cross sections

From the dependence of the deflection angle φ' on the impact parameter b, the differential scattering cross section $d\sigma/d\Omega$ could be calculated via (381). Since

the differential $d\sigma = 2\pi b \, db$ in (379) is the same in the lab and CM system, we need to change the expression for solid angle element $d\Omega$ by one for the lab system:

$$d\Omega_{\rm Lab} = 2\pi \sin \varphi \, d\varphi \,, \tag{405}$$

which leads to the simple relation between the differential scattering cross sections in the lab and the CM system,

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{Lab}} = \left(\frac{d\sigma}{d\Omega}\right)_{\text{CM}} \frac{\sin\varphi'}{\sin\varphi} \frac{d\varphi'}{d\varphi},$$
(406)

where the differential scattering cross sections are evaluated at corresponding angles φ in the lab, and φ' in the CM system. Evaluation of the correction factor on the right side of (406) is straightforward but a bit tedious; using (398), i.e.,

$$\tan \varphi = \frac{\sin \varphi'}{\cos \varphi' + \gamma} \tag{407}$$

one finds with $1/\tan^2 x = 1/\sin^2 x - 1$ first

$$\frac{\sin \varphi'}{\sin \varphi} = \sqrt{1 + \gamma^2 + 2\gamma \cos \varphi'}.$$
 (408)

Expressing the differential of (398) on the left side by $d\varphi$, and on the right side by $d\varphi'$ leads after some steps to

$$\frac{d\varphi'}{d\varphi} = \frac{1 + \gamma^2 + 2\gamma\cos\varphi'}{1 + \gamma\cos\varphi'},\tag{409}$$

and finally to a correction factor

$$\frac{\sin \varphi'}{\sin \varphi} \frac{d\varphi'}{d\varphi} = \frac{(1 + \gamma^2 + 2\gamma \cos \varphi')^{3/2}}{1 + \gamma \cos \varphi'} \tag{410}$$

8.6.4 Special cases

For the special case of elastic scattering (H=0), and $m_1=m_2$, one finds

$$\gamma = 1 \quad \text{and} \quad E' = E/2 \,, \tag{411}$$

SO

$$\tan \varphi = \frac{\sin \varphi'}{\cos \varphi' + 1} = \tan \frac{\varphi}{2}, \quad \text{or} \quad \varphi = \frac{\varphi'}{2}.$$
(412)

The correction factor (410) becomes

$$\frac{\sin \varphi'}{\sin \varphi} \frac{d\varphi'}{d\varphi} = 4\cos \varphi \,, \tag{413}$$

and

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{Lab}} = \left(\frac{d\sigma}{d\Omega}\right)_{\text{CM},\varphi'=2\varphi} \cdot 4\cos\varphi \,.$$
(414)

This case covers e.g. scattering of electrons electrons, or protons by protons.

The other important special case of elastic scattering (H = 0) is for a target mass m_2 much larger than the projectile mass m_1 . Then, $\gamma \approx 0$ and

$$\varphi' \approx \varphi$$
, $E' = E$, and $\left(\frac{d\sigma}{d\Omega}\right)_{\text{Lab}} = \left(\frac{d\sigma}{d\Omega}\right)_{\text{CM}, \varphi' = \varphi}$. (415)

This was the case for the classical Rutherford scattering experiment conducted by Geiger and Marsden¹⁴, where relatively light α particles ($m_1 = 4$ amu) were scattered of a thin foil of gold atoms ($m_2 \approx 197$ amu). The occasional relatively rare scattering of α particles in the backwards direction ($\varphi > 90^{\circ}$) indicated that the positive charge of the nuclei was localized in a very small space only, and not uniformly distributed over the whole size of the atom, as hypothesized by the then common "plum pudding" model of a large-sized positive charge to counterbalance the electrons.

¹⁴H. Geiger and E. Marsden, Proc. Roy. Soc. London A82, 495-500 (1909).

9 Harmonic oscillator

So far, we have encountered the undamped harmonic oscillator as an example for obtaining an equation of motion via various strategies, resulting in

$$F = m\ddot{x} = -kx \quad \text{or} \quad \ddot{x} + \omega_0^2 x = 0 \tag{416}$$

with $\omega_0^2 = k/m$ for the dynamical variable x, with oscillating solutions discussed in section 2.3.3. Since the harmonic oscillator is at the core of many dynamic phenomena in physics, it deserves a closer look, and the inclusion of dissipation as well as response to time-varying external forces.

9.1 Damped harmonic oscillator

First, we extend the basic model by a damping term. This can be thought of as a friction force present in the motion. In its simplest form (see section 2.3.2), the friction force would be proportional to the velocity \dot{x} of the system. This results in a modified equation of motion,

$$F = m\ddot{x} = -kx - \alpha \dot{x} \,, \tag{417}$$

or in the more commonly found form

$$\ddot{x} + 2\beta \dot{x} + \omega_0^2 x = 0, (418)$$

with $\beta > 0$ for a damping action. This is still a linear ordinary differential equation (ODE), and can also be solved using an exponential ansatz

$$x(t) = Ae^{rt}. (419)$$

Inserting this into (418) and division by x(t) leads to an algebraic equation for r,

$$r^2 + 2\beta r + \omega_0^2 = 0, (420)$$

which can easily be solved for its roots:

$$r_{1,2} = -\beta \pm \sqrt{\beta^2 - \omega_0^2} \,. \tag{421}$$

Depending on the values of ω_0 and β , the two roots $r_{1,2}$ can assume complex values. One distinguishes three cases for the solutions.

9.1.1 Underdamped case

If $0 < \beta < \omega_0$, the argument of the square root in (421) is negative, so r has an imaginary component:

$$r_{1,2} = -\beta \pm i\sqrt{\omega_0^2 - \beta^2} = -\beta \pm i\omega_1 \quad \text{with} \quad \omega_1 := \sqrt{\omega_0^2 - \beta^2}. \tag{422}$$

The corresponding solutions (419) are

$$x(t) = Ae^{-\beta t \pm i\omega_1 t} = Ae^{-\beta t}e^{\pm i\omega_1 t}. \tag{423}$$

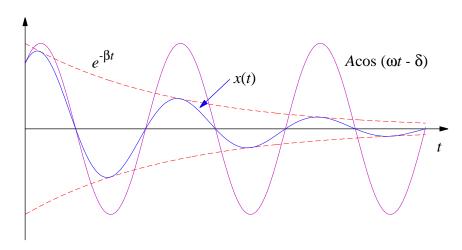
The first exponential provides the damping term that decays exponentially with time, while the second exponential forms an oscillating part, with an oscillation frequency ω_1 lower than the frequency ω_0 of the undamped system. As this is a second order differential equation, there are two integration constants that allow meeting the initial conditions of the problem; the most general solution to (418) can be written in various ways,

$$x(t) = (Ae^{i\omega_1 t} + A'e^{-i\omega_1 t})e^{-\beta t}$$

$$= (B\cos\omega_1 t + B'\sin\omega_1 t)e^{-\beta t}$$

$$= C\cos(\omega_1 t - \delta)e^{-\beta t}$$
(424)

for integration constant pairs (A, A'), (B, B'), or (C, δ) . The first form is convenient if complex parameters are to be considered, the second and third are often useful when a real-valued x(t) is expected. The solutions are illustrated below, where an oscillation of frequency $\omega_1 < \omega_0$ is multiplied with an exponentially decaying envelope $e^{-\beta t}$. For $t \to \infty$, the exponential term takes over, and $x(t) \to 0$.

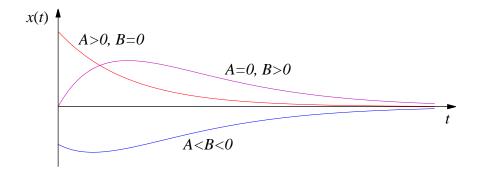


9.1.2 Critically damped case

For $\beta = \omega_0$, the two roots of (420) become degenerate, $r_{1,2} = -\beta$. In this case, one can verify that the ansatz

$$x(t) = (A + Bt) e^{-\beta t} \tag{425}$$

is a solution to (418), which can cover all initial conditions. Typical solutions for x(t) matching various initial conditions are shown below:



9.1.3 Overdamped case

For $\beta > \omega_0$, both roots $r_{1,2}$ in (421) are real and negative, because the square root

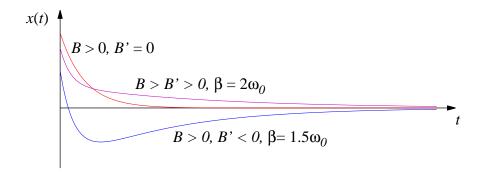
$$\sqrt{\beta^2 - \omega_0^2} =: \omega_2 \tag{426}$$

is always smaller than β . The solution for x(t) is a superposition of two exponential decays, with two time constants corresponding to r_1 and r_2 :

$$x(t) = (Ae^{\omega_2 t} + A'e^{-\omega_2 t})e^{-\beta t}$$

= $Be^{-(\beta + \omega_2)t} + B'e^{-(\beta - \omega_2)t}$. (427)

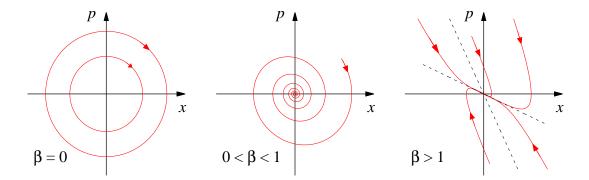
The figure below shows a few typical examples for x(t):



9.1.4 Damped oscillator trajectories in phase space

It is instructive to visualize the various cases for solutions to the harmonic oscillator problem in phase space. As introduced in section 7.2, the phase space for the simple harmonic oscillator is a plane with coordinates x and $p = mv = m\dot{x}$, i.e., the momentum is proportional to the speed of the oscillator.

On the left side of the figure below, the case $\beta = 0$ reproduces the closed elliptical trajectories we have seen in section 7.2. Various initial conditions lead to trajectories with different amplitude.



In the center, the underdamped case is illustrated for a single initial condition with a given amplitude and velocity. the trajectory is a logarithmic spiral, converging into the origin x = 0, p = 0 for $t \to \infty$.

On the right side, a few trajectories for the overdamped case are shown, with a fixed value $\beta = 1.3\omega_0$. The two dashed lines correspond to solutions of type (427) with either B = 0, or B' = 0 (fast decay or slow decay only). There, the ratio between position x and velocity \dot{x} is fixed and given by the respective decay rates $-\beta - \omega_2$ and $-\beta + \omega_2$. The trajectories first follow a direction corresponding to the faster decay rate $-\beta - \omega_2$. After some time, this contribution has become much smaller than the one with the slower decay rate $-\beta + \omega_2$, which then dominates how the trajectory approaches the origin of the phase space.

9.2 Harmonically driven harmonic oscillator

So far, we have only considered time-independent equations of motion, which are adequate for closed systems. However, physical systems are often driven by external forces, so it is important to know how the system responds. Staying with the (damped) harmonic oscillator, we first consider an external force $F_{\text{ext}}(t) = F_0 \cos(\omega t)$ with a harmonic time dependence:

$$\ddot{x} + 2\beta \dot{x} + \omega_0^2 x = A\cos(\omega t) \quad \text{with} \quad A = \frac{F_0}{m}. \tag{428}$$

This is a so-called *inhomogeneous* linear differential equation, with the inhomogeneity on the right side of the equation. The solution x(t) of such a differential equation is the sum of a *complementary solution* $x_c(t)$ to the homogeneous differential equation, as it was earlier presented in (424), (425), or (427), and a *particular solution* $x_p(t)$ that takes care of the sinusoidal driving part. We first solve this problem with a real-valued ansatz, and later with a complex-valued one. The first approach guarantees a real-valued solution, but the latter is algebraically simpler, and easier to derive and remember.

9.2.1 Solution with a real-valued ansatz

The inhomogeneity oscillates with a fixed (angular) frequency ω , so we expect a periodic solution x(t) with the same angular frequency. Similar to the ansatz in section 2.3.3, we allow for a phase shift δ and try

$$x(t) = B\cos(\omega t - \delta). \tag{429}$$

Direct differentiation and inserting into (428) leads to

$$-B\omega^2\cos(\omega t - \delta) - 2\beta B\omega\sin(\omega t - \delta) + \omega_0^2 B\cos(\omega t - \delta) = A\cos(\omega t). \quad (430)$$

This can be sorted into terms with sin and cos and rearranged:

$$(\omega_0^2 - \omega^2)\cos(\omega t - \delta) - 2\beta\omega\sin(\omega t - \delta) = \frac{A}{B}\cos(\omega t). \tag{431}$$

The oscillating terms with the phase shift δ on the left side can be expanded into an oscillating and a static part:

$$\cos(\omega t - \delta) = \cos \omega t \cos \delta + \sin \omega t \sin \delta$$

$$\sin(\omega t - \delta) = \sin \omega t \cos \delta - \cos \omega t \sin \delta$$
 (432)

With this, (431) can be arranged in a terms proportional to $\sin \omega t$ and $\cos \omega t$:

$$\left[(\omega_0^2 - \omega^2) \cos \delta + 2\beta \omega \sin \delta \right] \cos \omega t + \left[(\omega_0^2 - \omega^2) \sin \delta - 2\beta \omega \cos \delta \right] \sin \omega t = \frac{A}{R} \cos \omega t.$$
 (433)

Since this equation needs to hold for all times, the amplitude of the sin and cos components on both sides need to be the same, which leads to the two equations

$$(\omega_0^2 - \omega^2)\cos\delta + 2\beta\omega\sin\delta = \frac{A}{B}, \text{ and } (434)$$

$$(\omega_0^2 - \omega^2)\sin\delta - 2\beta\omega\cos\delta = 0. (435)$$

Equation (435) leads to an expression for the phase shift.

$$\tan \delta = \frac{2\beta\omega}{\omega_0^2 - \omega^2},\tag{436}$$

which provides expressions for $\sin \delta$ and $\cos \delta$ ':

$$\sin \delta = \frac{2\beta\omega}{\sqrt{(\omega_0^2 - \omega^2)^2 + 4\omega^2\beta^2}}$$
 and $\cos \delta = \frac{\omega_0^2 - \omega^2}{\sqrt{(\omega_0^2 - \omega^2)^2 + 4\omega^2\beta^2}}$. (437)

Those can be used to find a relationship between the amplitudes A of the driving acceleration, and the amplitude B of the resulting oscillation from (434):

$$\frac{B}{A} = \frac{1}{(\omega_0^2 - \omega^2)\cos\delta + 2\beta\omega\sin\delta} = \frac{1}{\sqrt{(\omega_0^2 - \omega^2)^2 + 4\omega^2\beta^2}}$$
(438)

Before we discuss the result, we show that by using complex amplitudes, the problem can be substantially simplified, without using relations for the trigonometric functions.

9.2.2 Solution with a complex-valued driving term

We first re-write the inhomogeneous differential equation (428) into one with a complex-valued inhomogeneity:

$$\ddot{x} + 2\beta \dot{x} + \omega_0^2 x = Ae^{i\omega t} \,. \tag{439}$$

Inserting the complex-valued ansatz

$$x_p(t) = Be^{i\omega t} (440)$$

into the differential equation (439) gives

$$-\omega^2 B e^{i\omega t} + 2i\beta \omega B e^{i\omega t} + \omega_0^2 B e^{i\omega t} = A e^{i\omega t}, \qquad (441)$$

leading to the algebraic equation

$$-\omega^2 + 2i\beta\omega + \omega_0^2 = \frac{A}{B} \tag{442}$$

or

$$\frac{1}{(\omega_0^2 - \omega^2) + 2i\beta\omega} = \frac{B}{A} =: \chi(\omega). \tag{443}$$

Here, we defined the *complex susceptibility* $\chi(\omega)$ which specifies the ratio between the amplitude B of the oscillator response, and the amplitude A of the driving oscillation. The modulus of the complex susceptibility is easy to calculate,

$$|\chi(\omega)| = \frac{1}{|(\omega_0^2 - \omega^2) + 2i\beta\omega|} = \frac{1}{\sqrt{(\omega_0^2 - \omega^2)^2 + 4\beta^2\omega^2}}$$
 (444)

and reproduces the result (438) for the amplitude ratio for a system driven by a real-valued harmonic inhomogeneity. Similarly, the argument $\arg(\chi)$ of the complex susceptibility reflects the phase shift between complex amplitudes B and A. For this, we remember that a complex number z can be written as

$$z = |z|e^{i\arg(z)}$$
 with $\tan(\arg(z)) = \frac{\operatorname{Im}[z]}{\operatorname{Re}[z]}$ (445)

With $1/(a+ib) = (a-ib)/(a^2+b^2)$, we find from (443)

$$\tan(\arg(\chi)) = \frac{-2\beta\omega}{\omega_0^2 - \omega^2} = \tan(-\delta), \qquad (446)$$

which reproduces the phase shift δ for the real-valued expression (436). The minus sign in the phase shift δ reflects the fact that we can write

$$x_n(t) = \chi(\omega) A e^{i\omega t} = A|\chi(\omega)|e^{-i\delta} e^{i\omega t} = A|\chi(\omega)|e^{i(\omega t - \delta)}, \qquad (447)$$

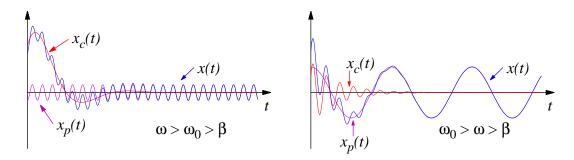
where a positive valued δ reflects a *phase lag* of the response with respect to the driving acceleration.

9.2.3 Transients in harmonically driven oscillators

As mentioned before, the solution x(t) to the harmonically driven oscillator is a linear combination of the particular solution we just obtained, and the complementary solution to the homogenous differential equation:

$$x(t) = x_c(t) + x_p(t). (448)$$

The complementary solution allows taking care of the initial conditions of the system, because the particular solution leaves no freedom to do so. For a time t long after the instant where the initial conditions were defined, the complementary solution $x_c(t)$ will have decayed for the damped harmonic oscillator, and the particular solution $x_p(t)$ will dominate the response. The complementary solution leads to a so-called *transient*, shown in the figure below for two examples:



9.2.4 Stationary solution of the driven harmonic oscillator

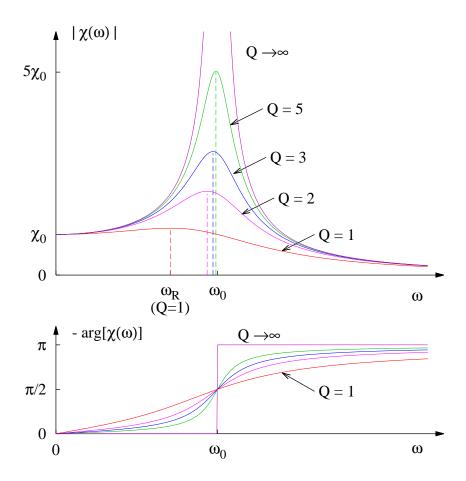
After the transients of the solution x(t) are gone, the system assumes the stationary solution $x_p(t)$, which is, apart from an amplitude, completely characterized by the complex susceptibility $\chi(\omega)$ from (443). With

$$\chi(\omega = 0) = \frac{1}{\omega_0^2} =: \chi_0. \tag{449}$$

and another customary definition of the so-called quality factor

$$Q := \frac{\omega_0}{2\beta} \tag{450}$$

that normalizes the damping factor β to the resonance frequency ω_0 of the undamped oscillator, the behavior of the susceptibility for different frequencies can then be discussed in a generic way. The modulus of the susceptibility, normalized to χ_0 and the phase shift $\delta = -\arg[\chi(\omega)]$ is shown in the following figure below for different values of Q.



The modulus $|\chi(\omega)|$ rises from χ_0 with increasing frequency to a single maximum at the resonance frequency $\omega = \omega_R$. The maximum is found by differentiating (444),

$$\frac{\partial |\chi(\omega)|}{\partial \omega} = \frac{-1/2}{\sqrt{(\omega_0^2 - \omega^2)^2 + 4\beta^2 \omega^2}} \left[2(\omega_0^2 - \omega^2)(-2\omega) + 8\omega\beta^2 \right]$$

$$= \frac{-2\omega}{\sqrt{\dots^3}} \left[\omega^2 - \omega_0^2 + 2\beta^2 \right] \stackrel{!}{=} 0$$
(451)

revealing the maximum at

$$\omega = \sqrt{\omega_0^2 - 2\beta^2} =: \omega_R. \tag{452}$$

This amplitude resonance frequency ω_R , the damped free oscillation frequency ω_1 , and the undamped oscillator frequency ω_0 obey the relation

$$\omega_0 > \omega_1 > \omega_R. \tag{453}$$

At $\omega = \omega_0$, the phase shift δ between driving force and oscillation amplitude has increased from 0 at $\omega = 0$ to $\delta = \pi/2$, i.e., the response of the oscillator on

resonance lags a quarter period behind to the driving force. The maximal value of the susceptibility modulus at the amplitude resonance ω_R takes the value

$$|\chi(\omega_R)| = \frac{1}{\sqrt{(\omega_0^2 - \omega_R^2)^2 + 4\beta^2 \omega_R^2}}$$

$$= \frac{1}{\sqrt{4\beta^4 + 4\beta^2 (\omega_0^2 - 2\beta^2)}} = \frac{1}{2\beta\sqrt{\omega_0^2 - \beta^2}} = \frac{1}{2\beta\omega_1}$$

$$= \frac{\chi_0 \omega_0^2}{2\beta\omega_0 \sqrt{1 - \beta^2/\omega_0^2}} = \frac{\chi_0 Q}{\sqrt{1 - 1/(4Q^2)}}.$$
(454)

For a weakly damped oscillator, $Q \gg 1$, so

$$\frac{|\chi(\omega_R)|}{\chi_0} \approx Q\,,\tag{455}$$

i.e., the resonance amplitude is increased by the factor of Q compared to the low frequency response at $\omega = 0$. For $\omega \gg \omega_0$,

$$|\chi(\omega)| \approx \frac{1}{\omega^2},$$
 (456)

and the phase lag approaches $\delta=\pi$, i.e., the response x(t) of the driven system is opposed to the driving force. The $1/\omega^2$ dependence is e.g. used to damp out high frequency vibrations on optical tables by making the table/suspension system an oscillator with a very low resonance frequency.

The resonance peak gets more pronounced for larger values of Q. To see this, we introduce a detuning $\Delta := \omega - \omega_0$ from the resonance, and approximate the susceptibility for $\Delta \ll \omega_0$:

$$|\chi(\omega)| = \frac{1}{\sqrt{(\omega + \omega_0)^2 (\omega - \omega_0)^2 + 4\beta^2 \omega^2}}$$

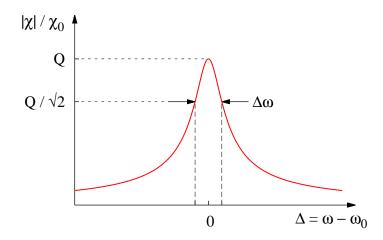
$$= \frac{1}{\sqrt{(2\omega_0 + \Delta)^2 \Delta^2 + \omega_0^2 / Q^2 (\omega_0 + \Delta)^2}}$$

$$\approx \frac{1}{\sqrt{4\omega_0^2 \Delta^2 + \omega_0^4 / Q^2}} = \frac{Q}{\omega_0^2 \sqrt{4Q^2 \Delta^2 / \omega_0^2 + 1}}$$

$$= \frac{\chi_0 Q}{\sqrt{4Q^2 \Delta^2 / \omega_0^2 + 1}}$$
(457)

This is the amplitude version of a so-called Lorentz profile, which governs resonance phenomena in many areas in physics, including spectral line of atoms and molecules.

One can assign a width $\Delta\omega$ of the resonance, defined by the frequency range where the average energy stored in the resonator exceeds half of the maximal



energy on resonance. Since the stored energy is proportional to x^2 and therefore proportional to $|\chi^2|$, we find the condition

$$\left| \chi \left(\omega_0 \pm \frac{\Delta \omega}{2} \right) \right| = \frac{Q}{\sqrt{2}} \quad \to \quad \Delta \omega = \frac{\omega_0}{Q}$$
 (458)

The maximum for the modulus of the susceptibility is located at

$$\omega_R = \sqrt{\omega_0^2 - 2\beta^2} = \omega_0 \sqrt{1 - \frac{1}{2Q^2}} \approx \omega_0 - \frac{\omega_0}{4Q^2} = \omega_0 - \frac{\Delta\omega}{4Q},$$
(459)

i.e., the peak separation from ω_0 is much smaller than the width $\Delta\omega$ of the resonance line for large Q. An example of mechanical resonators with $Q=10^4\dots 10^6$ are the quartz crystals forming the time basis of modern clocks.

9.3 Arbitrarily driven harmonic oscillator

In the previous section, we considered the harmonic oscillator with a sinusoidal or harmonic inhomogeneity, because of the simple temporal derivatives. The particular solution for the differential equation (439) with an inhomogeneity $Ae^{i\omega t}$ was

$$x_p(t) = \chi(\omega) A e^{i\omega t}, \qquad (460)$$

with a complex susceptibility $\chi(\omega)$ in (443). We now consider the more general equation of motion

$$\ddot{x} + 2\beta \dot{x} + \omega_0^2 x = a(t) \tag{461}$$

and start with an inhomogeneity that is a superposition of two harmonic terms,

$$a(t) = a_1 e^{i\Omega_1 t} + a_2 e^{i\Omega_2 t}. (462)$$

Note that the frequencies $\Omega_{1,2}$ can be arbitrary. Due to the linearity of the differential equation, the solution is the superposition of the solutions for the

individual harmonic driving terms,

$$x_p(t) = \chi(\Omega_1)a_1e^{i\Omega_1t} + \chi(\Omega_2)a_2e^{i\Omega_2t}.$$
 (463)

This also holds for a more general superposition and its corresponding solution,

$$a(t) = \sum_{n = -\infty}^{\infty} a_n e^{i\Omega_n t} \longrightarrow x_p(t) = \sum_{n = -\infty}^{\infty} a_n \chi(\Omega_n) e^{i\Omega_n t}. \tag{464}$$

For $\Omega_n = n \Omega_0$, the sum in a(t) is referred to as a Fourier series¹⁵. One can show that every square-integrable periodic function a(t) on an interval $[0, 2\pi/\Omega_0[$ can be expressed in this way¹⁶, and the coefficients a_n are uniquely determined by

$$a_n = \frac{\Omega_0}{2\pi} \int_{0}^{2\pi/\Omega_0} a(t) e^{-i n \Omega_0 t} dt.$$
 (465)

For non-periodic functions a(t) a similar transformation exists:

$$a(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{a}(\omega) e^{i\omega t} d\omega =: \mathcal{F}^{-1} \left[\tilde{a}(\omega) \right], \qquad (466)$$

which is the definition of the inverse Fourier transformation \mathcal{F}^{-1} for the continuous frequency distribution $\tilde{a}(\omega)$. This frequency distribution can be obtained via the direct Fourier transformation \mathcal{F} ,

$$\tilde{a}(\omega) = \mathcal{F}[a(t)] = \frac{1}{\sqrt{2\pi}} \int_{-2\pi}^{\infty} a(t) e^{-i\omega t} dt.$$
 (467)

The particular solution for an arbitrary inhomogeneity a(t) is therefore given by

$$x_p(t) = \mathcal{F}^{-1}\left[\tilde{x}(\omega)\right] = \mathcal{F}^{-1}\left[\chi(\omega)\tilde{a}(\omega)\right] = \mathcal{F}^{-1}\left[\chi(\omega)\mathcal{F}\left[a(t)\right]\right]. \tag{468}$$

This is a rather simple procedure: First, the Fourier transformation of the inhomogeneity a(t) is calculated, resulting in a Fourier distribution $\tilde{a}(\omega)$. The result is multiplied with the complex susceptibility $\chi(\omega)$, and the product transformed back to obtain $x_p(t)$.

This approach also takes care of the initial conditions $x(t \to -\infty) = 0$ and $\dot{x}(t \to -\infty) = 0$, so no complementary solution needs to be added.

 $^{^{15}}$ after Joseph Fourier, 1768-1830

¹⁶The right side of this interval is open to avoid problems with δ-functions on one of the interval limits - Fourier transformations work also for these rather strange functions.

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9.3.1 Examples of Fourier transformations

A commonly encountered function is a rectangular step function, with a height h and a width b, defined by

$$a(t) = \begin{cases} h & \text{for } |t| < b/2, \\ 0 & \text{elsewhere.} \end{cases}$$
 (469)

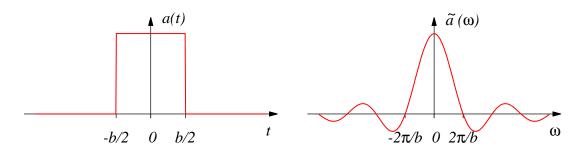
The Fourier transform of a(t) can directly be calculated:

$$\mathcal{F}[a(t)] = \tilde{a}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} a(t)e^{-i\omega t} dt = \frac{h}{\sqrt{2\pi}} \int_{-b/2}^{b/2} e^{-i\omega t} dt$$

$$= \frac{h}{\sqrt{2\pi}} \frac{1}{-i\omega} \left(e^{-i\omega b/2} - e^{+i\omega b/2} \right) = \frac{h}{\sqrt{2\pi}} \frac{2\sin(\omega b/2)}{\omega}$$

$$= \frac{hb}{\sqrt{2\pi}} \frac{\sin(\omega b/2)}{\omega b/2} = \frac{hb}{\sqrt{2\pi}} \operatorname{sinc}(\omega b/2). \tag{470}$$

The characteristic width of the real-valued function $\tilde{a}(\omega)$ in frequency space is inversely proportional to the width in real space:



Another example is the cosine function,

$$a(t) = \cos(\omega_0 t) = \frac{1}{2} \left(e^{i\omega_0 t} + e^{-i\omega_0 t} \right), \qquad (471)$$

with the rather simple Fourier transform

$$\tilde{a}(\omega) = \sqrt{\frac{\pi}{2}} \left(\delta(\omega - \omega_0) + \delta(\omega + \omega_0) \right) , \qquad (472)$$

which specializes for $\omega_0 = 0$ into

$$a(t) = 1 \quad \leftrightarrow \quad \tilde{a}(\omega) = \sqrt{2\pi} \,\delta(\omega) \,, \tag{473}$$

with the Dirac delta function $\delta(\omega)$.

9.3.2 Expression of the oscillator response with Green's function

While the solution of $x_p(t)$ for an arbitrary inhomogeneity a(t) is provided by (468), it is not very efficient in practice, because two integrations have to be carried out: one for the Fourier transformation, and one for the back transformation. The expression can be simplified by explicitly writing down both transformations, and then swapping integrations:

$$x_{p}(t) = \mathcal{F}^{-1} \left[\chi(\omega) \mathcal{F} \left[a(t) \right] \right]$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \, e^{i\omega t} \chi(\omega) \int_{-\infty}^{\infty} dt' \, e^{-i\omega t'} a(t')$$

$$= \int_{-\infty}^{\infty} dt' \, a(t') \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \, \chi(\omega) e^{i\omega(t-t')} \right]$$

$$= \int_{-\infty}^{\infty} dt' \, a(t') g(t-t') \quad \text{with} \quad g(\tau) := \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \, \chi(\omega) e^{i\omega\tau} \,. \tag{474}$$

For a given physical system like the damped harmonic oscillator, the function $g(\tau)$ needs to be evaluated only once, and the result can be used to obtain $x_p(t)$ from a(t) by a single integration. The combination of a(t) and g(t) in the form above is also referred to as a convolution of the two functions a(t) and g(t), which is also referred to as Green's function¹⁷ for the physical system.

Green's function has a simple physical interpretation. One rewrites the inhomogeneity a(t), and compares it with the response $x_p(t)$:

$$a(t) = \int_{-\infty}^{\infty} a(t')\delta(t - t') dt' \quad \to \quad x_p(t) = \int_{-\infty}^{\infty} a(t')g(t - t') dt'$$
 (475)

Using again the linearity of the differential equation (461), the function g(t-t') presents the response of the harmonic oscillator to a driving function $\delta(t-t')$, i.e., a delta pulse at time t'. An arbitrary function a(t) can be composed as a superposition of delta pulses according to the left side of (475). The response $x_p(t)$ of the system is an appropriately weighted superposition of the responses to these delta pulses. This idea behind Green's function carries over to many other areas in physics, especially in electromagnetism.

The task of determining g(t) for the harmonic oscillator can be solved in different ways:

- (a) directly by solving the differential equation (461) for a delta-shaped driving term, or
- (b) by carrying out the Fourier transformation of the complex susceptibility $\chi(\omega)$ according to the definition of g in (474).

¹⁷after George Green, 1793-1841

9.3.3 Green's function by direct integration

Green's function is the solution of the inhomogeneous differential equation

$$\ddot{x} + 2\beta \dot{x} + \omega_0^2 x = \delta(t), \qquad (476)$$

with initial conditions $x(-\epsilon) = 0$ and $\dot{x}(-\epsilon) = v(-\epsilon) = 0$ for a small $\epsilon > 0$ before the delta-shaped inhomogeneity. During the short impact at t = 0, the left side of (476) can be approximated by $\ddot{x}(t)$, because the system has not enough time to build up a significant speed or displacement. Therefore (476) becomes

$$\ddot{x} = \dot{v} \approx \delta(t) \,. \tag{477}$$

This can be directly integrated over a small region around the delta function,

$$\int_{-\epsilon}^{+\epsilon} \dot{v}(t) dt = \int_{-\epsilon}^{+\epsilon} \delta(t) dt = 1 \quad \to \quad v(\epsilon) - \underbrace{v(-\epsilon)}_{=0} = 1 \quad \text{or} \quad v(\epsilon) = 1. \tag{478}$$

The solution x(t) for $t > \epsilon$ can therefore be found by solving the homogenous differential equation with initial conditions x(0) = 0 and $\dot{x}(0) = 1$. We have done this already in (424). Assuming we have a case $\beta < \omega_0$, we choose the form

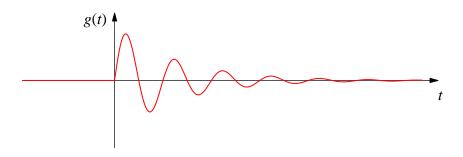
$$x(t) = \left[B\cos(\omega_1 t) + B'\sin(\omega_1 t)\right]e^{-\beta t}.$$
 (479)

The initial condition x(0) = 0 implies that B = 0. To meet the second initial condition, we calculate the speed

$$\dot{x} = B' \left[\cos(\omega_1 t) \omega_1 e^{-\beta t} + \sin(\omega_1 t) (-\beta) e^{-\beta t} \right] \quad \text{or} \quad \dot{x}(0) = B' \omega_1 \tag{480}$$

and find $B' = 1/\omega_1$, which completes the solution x(t). For t < 0, we demand x(t) = 0. Therefore, Green's function for the damped harmonic oscillator is

$$g(t) = \begin{cases} \frac{1}{\omega_1} e^{-\beta t} \sin(\omega_1 t) & \text{for } t > 0, \\ 0 & \text{for } t \le 0. \end{cases}$$
 (481)

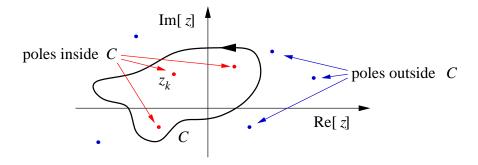


9.3.4 Green's function from Fourier transformation of $\chi(\omega)$

From the definition in (474), it follows that Green's function is essentially the (inverse) Fourier transform of the complex susceptibility:

$$g(\tau) = \frac{1}{\sqrt{2\pi}} \mathcal{F}^{-1} \left[\chi(\omega) \right] = \frac{1}{2\pi} \int_{-\infty}^{\infty} \chi(\omega) e^{i\omega\tau} d\omega =: \frac{1}{2\pi} \int_{-\infty}^{\infty} f(\omega) d\omega \qquad (482)$$

Such integrations can be carried out efficiently by making use of a result from complex calculus. Cauchy's *residue theorem*¹⁸ considers the integral of a function f(z) along a closed path C in the complex plane:



The theorem states that the integral of f(z) along C (when evaluated in counterclockwise direction) is given by

$$\oint_C f(z) dz = 2\pi i \sum_{z_k} \text{Res}(f, z_k), \qquad (483)$$

where z_k are the *poles* of the function f(z) (i.e., locations where f(z) diverges) inside the path C, and $Res(f, z_k)$ the so-called *residues* of f at the poles z_k . Poles outside the path C do not contribute to the integral. A residue at z_k is defined as element f_{-1} in the Laurent expansion

$$f(z) = \sum_{n=-\infty}^{\infty} f_n (z - z_k)^n$$
(484)

around the position z_k of a pole. This *Laurent series*¹⁹ is an extension of the *Taylor series* (where $n = 0...\infty$) to functions with a singularity/pole.

To use this theorem, we first extend the kernel of the integral (482) to a complex-valued parameter z:

$$f(\omega) = \chi(\omega) e^{i\omega\tau} \quad \to \quad f(z) = \frac{e^{iz\tau}}{\omega_0^2 - z^2 + 2iz\beta}$$
 (485)

¹⁸after Augustin-Louis Cauchy, French mathematician, 1789-1857

¹⁹ after P.A. Laurent, French mathematician, 1813-1854

The denominator of f(z) vanishes at two complex locations

$$z_{a,b} = i\beta \pm \sqrt{\omega_0^2 - \beta^2} = i\beta \pm \omega_1, \qquad (486)$$

where f(z) will have poles:

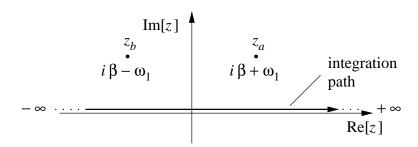
$$f(z) = \frac{-e^{iz\tau}}{(z - z_a)(z - z_b)}. (487)$$

The minus sign reflects that the z^2 term in the denominator of (485) is negative. The two residues of f are the respective parts that remain when leaving out the divergent factor $1/(z-z_a)$ or $1/(z-z_b)$:

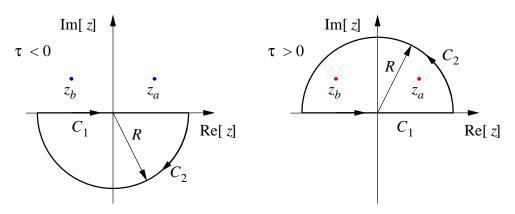
$$\operatorname{Res}[f, z_{a}] = \frac{-e^{iz_{a}\tau}}{(z_{a} - z_{b})} = \frac{-e^{-\beta\tau} e^{i\omega_{1}\tau}}{2\omega_{1}}$$

$$\operatorname{Res}[f, z_{b}] = \frac{-e^{iz_{b}\tau}}{(z_{b} - z_{a})} = \frac{e^{-\beta\tau} e^{-i\omega_{1}\tau}}{2\omega_{1}}$$
(488)

The location of the poles of f is shown in the diagram below, together with the integration path from $z = -\infty$ to $z = +\infty$ along the real axis for (482):



In a next step, the integration along the real axis needs to be translated into an integration along a closed path C. For this, we construct C from a part C_1 along the real axis from z = -R to z = +R, and a semicircle C_2 with radius R:



For $R \to \infty$, the integral along C_1 will become the integral in (482) for $g(\tau)$, and we show that integral I_2 along the semicircle C_2 vanishes. To do so, we parameterize C_2 by an angle ϕ and the radius R:

$$z = Re^{i\phi}$$
 \rightarrow $I_2 = \int_{C_2} f(z) dz = \int_{C_2} f(Re^{i\phi}) \frac{dz}{d\phi} d\phi$. (489)

To show that I_2 vanishes, it is enough to consider the modulus of the integral:

$$|I_{2}| = \left| \int_{C_{2}} \frac{-e^{iR(\cos\phi + i\sin\phi)\tau}}{(z - z_{a})(z - z_{b})} iRe^{i\phi} d\phi \right|$$

$$\leq \int_{C_{2}} \left| \frac{-e^{iR(\cos\phi + i\sin\phi)\tau}}{(z - z_{a})(z - z_{b})} iRe^{i\phi} \right| d\phi = \int_{C_{2}} \frac{R e^{-R\tau\sin\phi}}{|(z - z_{a})(z - z_{b})|} d\phi \quad (490)$$

For z on the semicircle with a radius R large enough to include the poles,

$$|z - z_{a,b}| > R - \sqrt{\omega_1^2 + \beta^2} = R - \omega_0,$$
 (491)

and therefore

$$|I_2| \le \int_{C_2} \frac{R e^{-R\tau \sin \phi}}{|(z - z_a)(z - z_b)|} d\phi < \frac{R}{(R - \omega_0)^2} \int_{C_2} e^{-R\tau \sin \phi} d\phi.$$
 (492)

For $\tau < 0$, we choose the bottom semicircle shown in the left part of the figure. There, $\sin \phi \leq 0$, so $e^{-R\tau \sin \phi} \leq 1$ so

$$|I_2| < \frac{R}{(R-\omega_0)^2} \int_{C_2} e^{-R\tau \sin\phi} d\phi \le \frac{R}{(R-\omega_0)^2} \int_{C_2} d\phi = \frac{R\pi}{(R-\omega_0)^2}.$$
 (493)

The last upper bound for I_2 vanishes for $R \to \infty$, so

$$\lim_{R \to \infty} |I_2| < \lim_{R \to \infty} \frac{R \pi}{(R - \omega_0)^2} = 0 \quad \Rightarrow \quad \lim_{R \to \infty} I_2 = 0. \tag{494}$$

There are no poles surrounded by C in the lower imaginary plane, so

$$g(\tau < 0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(\omega) d\omega = \frac{1}{2\pi} \lim_{R \to \infty} \int_{C_1} f(z) dz = \frac{1}{2\pi} \lim_{R \to \infty} \oint_{C} f(z) dz = 0.$$
 (495)

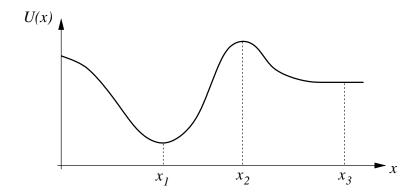
For $\tau > 0$, the same argument holds for the vanishing contribution from C_2 in the *upper semiplane*. The full path C now encloses the two poles at z_a and z_b , so

$$g(\tau > 0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(\omega) d\omega = \frac{1}{2\pi} \lim_{R \to \infty} \int_{C_1} f(z) dz = \frac{1}{2\pi} \lim_{R \to \infty} \oint_{C} f(z) dz$$
$$= \frac{1}{2\pi} 2\pi i \left(\operatorname{Res}[f, z_a] + \operatorname{Res}[f, z_b] \right)$$
$$= i \left(\frac{-e^{-\beta \tau} e^{i\omega_1 \tau}}{2\omega_1} + \frac{e^{-\beta \tau} e^{-i\omega_1 \tau}}{2\omega_1} \right)$$
$$= \frac{1}{\omega_1} e^{-\beta \tau} \sin \omega_1 \tau. \tag{496}$$

This reproduces the result we found by direct integration in (481).

9.4 Small oscillations

The concept of the harmonic oscillator and its associated solutions in the presence of damping and external excitation can be found in many physical situations, and may apply even where a restoring force is only approximately linear in the respective coordinate. We consider an arbitrary potential for a system with a single degree of freedom, describing the conservative interaction with its environment:



The potential U(x) shall have a minimum at position x_1 . For small deviations u from x_1 , the potential can be approximated by a Taylor expansion:

$$U(x) = U(x_1) + \underbrace{\frac{\partial U}{\partial x}\Big|_{x=x_1}}_{=0} u + \frac{1}{2} \frac{\partial^2 U}{\partial x^2}\Big|_{x=x_1} u^2 + \dots, \quad \text{with } u = (x - x_1)$$
(497)

In a minimum of U(x), the second term vanishes by definition, and the potential resembles that of a harmonic oscillator, since the constant offset $U(x_1)$ does not change the dynamics of the system.

The minimum is characterized by a positive second derivative of the potential,

$$\left. \frac{\partial^2 U}{\partial x^2} \right|_{x=x_1} > 0, \tag{498}$$

leading to the oscillatory solutions of the harmonic oscillator.

In presence of a damping force, a system starting near x_1 with a low enough velocity will approach x_1 asymptotically in time. Therefore, such a position is referred to as a *stable equilibrium*. For a maximum in the potential energy, like at position x_2 in the graph above, the second derivative is negative, which does not lead to an oscillatory motion. While a particle at rest at x_2 will stay there for all times, any small deviation will lead to a trajectory that starts with an exponentially growing separation from x_2 .

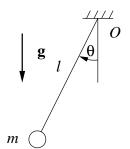
As most of the physical systems will experience small fluctuations of forces, and some dissipation, system tend to evolve into a state near a minimum where $\partial^2 U/\partial x^2 > 0$, which is therefore also referred to as a *stable equilibrium*. A

position where the potential energy takes a maximum, or $\partial^2 U/\partial x^2 < 0$ is referred to as an unstable equilibrium. To complete the description, a location like x_3 where $\partial^2 U/\partial x^2 = 0$ over some extended interval is referred to as an indifferent equilibrium. It should be pointed out that a minimum or maximum could still be present, but the second derivative could vanish. In that case, the sign of the first non-vanishing term in the Taylor expansion of U(x) would determine if the equilibrium is stable or unstable, but such situations are very rare in practice.

Therefore, the small deviations of a system from a stable equilibrium can often be mapped to a harmonic oscillator, assuming the kinetic energy is of a quadratic form in the velocity \dot{x} . As the restoring force $F = -\partial U/\partial x$ near a minimum is linear in the deviation u, this procedure is sometimes referred to as linearization.

9.4.1 Example of the plane pendulum

As a simple example, we revisit the plane pendulum from section 6.2.1:



$$U = mgl (1 - \cos \theta),$$

$$T = \frac{1}{2} ml^2 \dot{\theta}^2,$$
 (499)

leading to the nonlinear differential equation (199)

$$\ddot{\theta} + \frac{g}{I}\sin\theta = 0. \tag{500}$$

A Taylor expansion of the potential near the minimum at $\theta = 0$ leads to

$$U(\theta) \approx \frac{1}{2} \, mgl \, \theta^2 \,, \tag{501}$$

and an approximate Lagrange function of

$$L = T - U = \frac{1}{2} m l^2 \dot{\theta}^2 - \frac{1}{2} m g l \theta^2, \qquad (502)$$

which after some simplification leads to the equation of motion

$$\ddot{\theta} + \frac{g}{l}\theta = 0. \tag{503}$$

This is the equation of motion for the undamped harmonic oscillator, and by comparison e.g. with (418), one can immediately extract the oscillation frequency

$$\omega_0 = \sqrt{\frac{g}{l}} \,. \tag{504}$$

10 Coupled oscillations

So far, we have encountered methods to generate equations of motion for system of many particles, but have not really solved very complex systems. In this section, we will look into a typical system of many harmonic oscillators. Such a problem may arise from a system of particles near an equilibrium that are coupled together by some localized interactions, and can be approximated by harmonic oscillators as seen in section 9.4.

10.1 Two coupled oscillators

We demonstrate the strategy to tackle coupled oscillator problems with that of two masses, coupled by springs:

The equations of motion can be obtained in various ways, and form a system of *coupled* differential equations:

$$m \ddot{x}_1 + k_1 x_1 + k_{12} (x_1 - x_2) = 0$$

$$m \ddot{x}_2 + k_2 x_2 + k_{12} (x_2 - x_1) = 0$$
(505)

The coupling means that these are not independent equations of motion for x_1 and x_2 , and we need to find a solution for both variables that satisfy both equations at the same time. As these equations are still linear, we can try the previous trick, and look for complex solutions of the form

$$x_1(t) = b_1 e^{i\omega t}, \quad x_2(t) = b_2 e^{i\omega t},$$
 (506)

with the same oscillation frequency ω for both variables, but different complex amplitudes b_1 , b_2 . Inserting these into (505) leads to

$$\left(-m\omega^2 b_1 + (k_1 + k_{12})b_2 - k_{12}b_1 \right) e^{i\omega t} = 0$$

$$\left(-m\omega^2 b_2 + (k_2 + k_{12})b_1 - k_{12}b_2 \right) e^{i\omega t} = 0.$$
(507)

As before, we can divide by the exponential function, and obtain an algebraic equation determining the oscillation frequency. This time, however, the two equations remain coupled via the amplitudes. The algebraic equation is linear in the b, and can be written in matrix form,

$$\begin{pmatrix} -m\omega^2 + (k_1 + k_{12}) & -k_{12} \\ -k_{12} & -m\omega^2 + (k_2 + k_{12}) \end{pmatrix} \cdot \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = 0, \quad (508)$$

or simply

$$\underline{\mathbf{M}} \cdot \mathbf{b} = 0, \tag{509}$$

where the symbol $\underline{\underline{\mathbf{M}}}$ denotes a matrix, and \mathbf{b} a vector that is made up by two amplitudes. Note that this is now a vector that does not represent a vector in the usual three-dimensional space, it just stores the coefficients. The condition for this matrix equation to be fulfilled is

$$\det \underline{\mathbf{M}} = 0, \tag{510}$$

which leads to the characteristic equation of the linear equation system (508)

$$\left[-m\omega^2 + (k_1 + k_{12})\right] \left[-m\omega^2 + (k_2 + k_{12})\right] - k_{12}^2 = 0.$$
 (511)

To simplify the subsequent treatment, we assume now that $k_1 = k_2 = k$, so the characteristic equation becomes

$$(k + k_{12} - m\omega^2)^2 - k_{12}^2 = 0, (512)$$

which can easily be resolved for the two roots for ω ,

$$\omega_{1,2} = \sqrt{\frac{k + k_{12} \pm k_{12}}{m}} \quad \text{or} \quad \omega_1 = \sqrt{\frac{k + 2k_{12}}{m}}, \quad \omega_2 = \sqrt{\frac{k}{m}}.$$
(513)

As with the simple harmonic oscillator, we can have solutions with both signs for ω , and the general solution of the system (508) would be given by

$$x_{1}(t) = b_{11}^{+}e^{i\omega_{1}t} + b_{11}^{-}e^{-i\omega_{1}t} + b_{12}^{+}e^{i\omega_{2}t} + b_{12}^{-}e^{-i\omega_{2}t}$$

$$x_{2}(t) = b_{21}^{+}e^{i\omega_{1}t} + b_{21}^{-}e^{-i\omega_{1}t} + b_{22}^{+}e^{i\omega_{2}t} + b_{22}^{-}e^{-i\omega_{2}t}.$$
(514)

Here, the indices on b indicate the mass index, and the frequency of the system. However, these eight coefficients are not independent - they still need to fulfill (508), which imposes a relation between the amplitudes for the two masses. Inserting the solutions (514), and restricting to either positive or negative frequencies yields

for
$$\omega = \omega_1$$
: $-k_{12}b_{11} - k_{12}b_{21} = 0 \rightarrow b_{11} = -b_{21} =: B_1$,
for $\omega = \omega_2$: $+k_{12}b_{12} - k_{12}b_{22} = 0 \rightarrow b_{12} = b_{22} =: B_2$. (515)

The general solution of the coupled problem is then given by

$$x_1(t) = B_1^+ e^{i\omega_1 t} + B_1^- e^{-i\omega_1 t} + B_2^+ e^{i\omega_2 t} + B_2^- e^{-i\omega_2 t}$$

$$x_2(t) = -B_1^+ e^{i\omega_1 t} - B_1^- e^{-i\omega_1 t} + B_2^+ e^{i\omega_2 t} + B_2^- e^{-i\omega_2 t},$$
(516)

with four constants B_1^+ , B_1^- , B_2^+ , B_2^- to satisfy the initial conditions of the problem — the system is hereby completely determined, as (508) is a system of differential equations of second order.

10.1.1 Normal coordinates

The system has two oscillation frequencies ω_1 and ω_2 , and both masses participate in oscillations at those two frequencies. One can ask for coordinates that simplify the description of the problem. To see that this is the case, we define coordinates

$$\eta_1 := x_1 - x_2, \quad \text{and} \quad \eta_2 := x_1 + x_2,$$
(517)

such that the original coordinates can be obtained again via

$$x_{1,2} = \frac{1}{2}(\eta_2 \pm \eta_1). \tag{518}$$

Inserting this into the coupled equations of motion (505) leads to

$$\frac{m}{2}(\ddot{\eta}_2 + \ddot{\eta}_1) + \frac{k}{2}(\eta_2 + \eta_1) + k_{12}\eta_1 = 0$$

$$\frac{m}{2}(\ddot{\eta}_2 - \ddot{\eta}_1) + \frac{k}{2}(\eta_2 - \eta_1) - k_{12}\eta_1 = 0$$
(519)

This system of equations can be transformed into another one by subtracting and adding the two equations,

$$m \ddot{\eta}_1 + (k+2k_{12}) \eta_1 = 0$$

 $m \ddot{\eta}_2 + k \eta_2 = 0.$ (520)

This is now a *decoupled* system of two equations of two independent harmonics oscillators. Their solutions can be simply written from (69) as

$$\eta_1(t) = C_1^+ e^{i\omega_1 t} + C_1^- e^{-i\omega_1 t},
\eta_2(t) = C_2^+ e^{i\omega_2 t} + C_2^- e^{-i\omega_2 t}.$$
(521)

Coordinates η_1 and η_2 for this system are referred to as *normal coordinates*, a name that is justified in a later section. By appropriate choice of initial conditions, one can ensure that only one of the coordinates has a non-trivial solution. For example, if we choose

$$x_1(0) = -x_2(0)$$
 and $\dot{x}_1(0) = -\dot{x}_2(0)$, (522)

we know from (517) that

$$\eta_2(0) = 0 \quad \text{and} \quad \dot{\eta}_2(0) = 0,$$
(523)

and we will find an oscillation with a single frequency ω_1 . For this solution, the two amplitudes x_1 and x_2 are always related via

$$x_1(t) = -x_2(t), (524)$$

i.e., the two masses move *out of phase* or in an antisymmetric oscillation; occasionally this mode of oscillation is also referred to as a *breathing mode*. Similarly, if initial conditions are chosen such that

$$x_1(0) = x_2(0)$$
 and $\dot{x}_1(0) = \dot{x}_2(0)$, (525)

an oscillation takes place only at a frequency ω_2 , with

$$x_1(t) = x_2(t) (526)$$

at all times. This mode of oscillation is a symmetric mode, and some times referred to as *common mode oscillation*.

Both oscillation modes with only one frequency appearing can be understood as an effective one-variable problem: For the antisymmetric mode, the individual masses oscillate independently between two springs and a fixed center position of the middle spring, leading to a larger effective spring constant for the single mass motion. For the symmetric case, the inner spring stays always in its equilibrium position, and the only restoring force to the masses motion is provided by the outside springs, leading to the same result as we have seen from the simple mass/spring system in section 2.3.3.

10.1.2 Beat of oscillations

Before we move on to a more general treatment of coupled systems, we consider the special case where the coupling constant k_{12} between the two masses is much smaller than the other spring constants k. Then, the two oscillation frequencies $\omega_{1,2}$ from (513) become very similar, and one can define

$$\omega_0 := \frac{\omega_1 + \omega_2}{2}, \quad \text{and} \quad \Delta := \frac{\omega_1 - \omega_2}{2},$$

$$(527)$$

with $\omega_0 \gg \Delta$. If we further assume the initial conditions

$$x_1(0) = D$$
, $x_2(0) = 0$, $\dot{x}_1(0) = \dot{x}_2(0) = 0$, (528)

i.e., the system starts with only one mass displaced from its resting position, the coefficients in (516) become

$$B_1^+ = B_1^- = B_2^+ = B_2^- = \frac{D}{4}.$$
 (529)

The oscillation of mass 1 over time can be written as

$$x_1(t) = \frac{D}{4} \left[e^{i\omega_1 t} + e^{-i\omega_1 t} + e^{i\omega_2 t} + e^{-i\omega_2 t} \right]$$

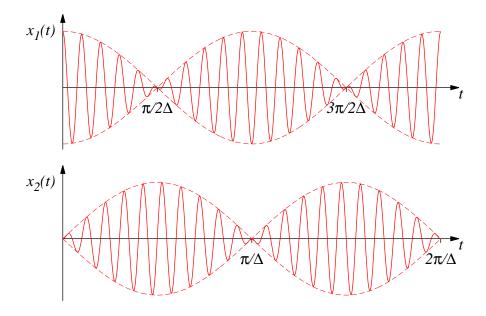
$$= \frac{D}{4} \left(2\cos(\omega_1 t) + 2\cos(\omega_2 t) \right)$$

$$= D\cos\left[\frac{\omega_1 + \omega_2}{2} \right] \cos\left(\frac{\omega_1 - \omega_2}{2} \right) = D\cos(\omega_0 t) \cos(\Delta t). \quad (530)$$

Similarly, one obtains for the oscillation of mass 2 the expression

$$x_2(t) = D\sin(\omega_0 t)\sin(\Delta t). \tag{531}$$

Qualitatively, the oscillation of the system looks as shown below:



Initially, mass 1 oscillates with approximate frequency ω_0 , and mass 2 is at rest. Then, the oscillation of mass 1 decreases in amplitude, while the amplitude of mass 2 increases. At time $t = \pi/2\Delta$, only mass 2 oscillates, before the pattern reverses, and mass 1 increases its amplitude again. This phenomenon is referred to as a *beat* of two oscillations, and can be found in many weakly coupled oscillators of the same frequency. The dashed lines in the figure above indicate the envelope of the oscillations.

10.2 Many coupled particles – small oscillations

In this section, we try to extend the idea of small oscillations to a system of many particles, e.g. molecules or the even more complex solids, where many atoms are hold together by chemical bonds, which are not completely rigid. However, the approach we take is not limited to these special situations, and goes also beyond mechanics.

We start with a system described by N generalized coordinates, forming the set $\{q_k\}$. The interactions should be conservative, i.e., they can be described by a single potential $U(\{q_k\})$. We now assume that the system is near an equilibrium state, possibly due to the presence of some dissipating forces which we exclude in the treatment. The equilibrium position of all coordinates shall be given by the set $\{q_{k,0}\}$. Similar to the simple one-dimensional problem in section 9.4, we

can approximate the potential U by a truncated Taylor expansion. This time, however, we need to do the Taylor expansion for N coordinates:

$$U(\{q_{k}\}) = \underbrace{U(\{q_{k,0}\})}_{=:U_{0}} + \sum_{k} \underbrace{\frac{\partial U}{\partial q_{k}} \Big|_{0}}_{=-\phi_{k}} (q_{k} - q_{k,0}) + \sum_{j,k} \frac{\partial^{2} U}{\partial q_{j} \partial q_{k}} \Big|_{0} \frac{1}{2} (q_{k} - q_{k,0}) (q_{j} - q_{j,0}) + \dots$$
(532)

The first term is simply the constant potential energy U_0 in the equilibrium, and will not be relevant for the dynamics of the system. In the second term, the first derivative of of the potential corresponds to the generalized force ϕ_k (see section 6.5). These forces are evaluated at the equilibrium position $\{q_{k,0}\}$ of the system, where they vanish by definition. By introducing variables

$$u_k := q_k - q_{k,0} \tag{533}$$

for the displacement of coordinate k from the equilibrium position, we can formulate the approximate potential energy by the first non-vanishing and relevant term in these displacements:

$$U = U_0 + \frac{1}{2} \sum_{j,k} A_{jk} u_j u_k , \quad \text{with} \quad A_{jk} := \frac{\partial^2 U}{\partial q_j \partial q_k} \bigg|_0 , \qquad (534)$$

where the index 0 at the second derivative in A_{jk} indicates again that it has to be taken at the equilibrium position set $\{q_{k,0}\}$. Since the sequence of the differentiation does not matter, we have the symmetry

$$A_{jk} = A_{kj}. (535)$$

We now try a similar expansion for the kinetic energy T of the system. Here, we recall from (238) in section 6.4 that for time-independent transformations from Cartesian to generalized coordinates, the total kinetic energy can be written as

$$T = \sum_{j,k} a_{jk} \dot{q}_j \dot{q}_k \quad \text{with} \quad a_{jk} = \frac{1}{2} \sum_{\alpha} m_{\alpha} \sum_{i} \frac{\partial x_{\alpha,i}}{\partial q_k} \frac{\partial x_{\alpha,i}}{\partial q_j}, \tag{536}$$

where the summations in the definition of a_{jk} go over all particles α and Cartesian coordinates i. Since the a_{jk} still can depend on the coordinates, we also perform a Taylor expansion,

$$a_{jk} = a_{jk}|_{0} + \sum_{l} \frac{\partial a_{jk}}{q_{l}}|_{0} (q_{l} - q_{l,0}) + \dots$$
 (537)

In this expansion, the first term *does not* vanish, so we stop right there (even neglecting the linear term), and define

$$m_{jk} := 2 |a_{jk}|_0 . (538)$$

These coefficients do not depend on the deviations u_k anymore. Because the sequence of the differentiations in a_{jk} does not matter, we also have $m_{jk} = m_{kj}$. With $\dot{q}_k = \dot{u}_k$, the kinetic energy can then be written as

$$T = \frac{1}{2} \sum_{j,k} m_{jk} \dot{u}_j \dot{u}_k \,. \tag{539}$$

The Lagrange function for small deviations from the equilibrium position becomes

$$L = T - U = \frac{1}{2} \sum_{i,j} \left[m_{ij} \dot{u}_i \dot{u}_j - A_{ij} u_i u_j \right] - U_0,$$
 (540)

with constant coefficients m_{ij} and A_{ij} . This expression has bilinear terms in the new coordinates u_k , and bilinear terms in the velocities \dot{u}_k — a structure very similar to a harmonic oscillator. The resulting equations of motion are obtained via the Euler-Lagrange method:

$$\frac{\partial L}{\partial u_k} - \frac{d}{dt} \frac{\partial L}{\partial \dot{u}_k} = -\sum_j A_{jk} u_j - \frac{d}{dt} \sum_j m_{jk} \dot{u}_j = 0, \qquad (541)$$

or

$$\sum_{j} \left[m_{jk} \ddot{u}_j + A_{jk} u_j \right] = 0 \quad \text{for all } k.$$
 (542)

This set of equations can be written as a matrix equation,

$$\underline{\mathbf{m}} \cdot \ddot{\mathbf{u}}(t) + \underline{\mathbf{A}} \cdot \mathbf{u}(t) = 0, \qquad (543)$$

where $\underline{\mathbf{m}}$ is the mass matrix, $\underline{\underline{\mathbf{A}}}$ is a matrix that describes the elastic response of a system, and \mathbf{u} is a vector made up by all the displacement coordinates u_k in the system.

10.2.1 Solving the equations of motion

We can solve equation (543) in the same way as in section 2.3.3, e.g. with a harmonic ansatz

$$\mathbf{u}(t) = \mathbf{a}\cos(\omega t - \delta)$$
, or componentwise: $u_k(t) = a_k\cos(\omega t - \delta)$, (544)

leading to an algebraic set of equations

$$(\underline{\mathbf{A}} - \omega^2 \underline{\mathbf{m}}) \cdot \mathbf{a} = 0 \tag{545}$$

or componentwise:
$$\sum_{i} (A_{kj} - \omega^2 m_{kj}) a_j = 0 \,\forall_k$$
, (546)

with constant amplitude coefficients a_k forming a vector **a**. This is again a set of algebraic equations, with a condition

$$\det\left(\underline{\underline{\mathbf{A}}} - \omega^2 \underline{\underline{\mathbf{m}}}\right) \stackrel{!}{=} 0 \tag{547}$$

to have solutions. This characteristic or secular equation for the ω^2 has N roots, where N is the number of coordinates in the system. The resulting frequencies $\omega_r, r = 1 \dots N$ are referred to as *eigenfrequencies* or characteristic frequencies of the problem.

For each eigenfrequency ω_r , a vector \mathbf{a}_r of amplitude coefficients solves the equation set (545). These vectors characterize the modes of oscillation, i.e., the relative amplitude with which each coordinate oscillates at this particular frequency. That mode of oscillation is also referred to as *eigenmode* for an oscillation at frequency ω_r . With this, the general solution of the coupled oscillation can be written as

$$\mathbf{u}(t) = \sum_{r=1}^{N} \alpha_r \mathbf{a}_r \cos(\omega_r t - \delta_r), \qquad (548)$$

with a factor α_r permitting normalization of \mathbf{a}_r , or componentwise

$$u_k(t) = \sum_{r=1}^{N} \alpha_r a_{k,r} \cos(\omega_r t - \delta_r), \qquad (549)$$

with real-valued amplitudes $\alpha_r \mathbf{a}_r$ and phase shifts δ_r for the contributions of the various eigenmodes to the oscillation. In the componentwise expression, the elements $a_{k,r}$ are the k-th component of eigenvector \mathbf{a}_r .

It is interesting to investigate some properties of the vector \mathbf{a}_r that characterizes a particular eigenmode. Since it has to fulfill (545), it is not completely determined, and any vector $\alpha \mathbf{a}_r$ would also fulfill that equation. One can therefore choose the normalization of the vector such that

$$\mathbf{a}_r \cdot (\underline{\underline{\mathbf{m}}} \cdot \mathbf{a}_r) = 1. \tag{550}$$

In this expression, the term in the parenthesis is a vector multiplied from the right to a matrix, leading to another vector. This vector then gets multiplied with another vector via a scalar product, leading to a scalar result 1. Furthermore, vectors \mathbf{a}_r and \mathbf{a}_s fulfill a generalized orthogonality relation²⁰:

$$\mathbf{a}_r \cdot \underline{\mathbf{m}} \cdot \mathbf{a}_s = 0 \quad \text{for} \quad r \neq s \,.$$
 (551)

To see this, we take two solutions of (545) for different eigenfrequencies,

$$\omega_r^2 \underline{\underline{\mathbf{m}}} \cdot \mathbf{a}_r = \underline{\underline{\mathbf{A}}} \cdot \mathbf{a}_r \omega_s^2 \underline{\underline{\mathbf{m}}} \cdot \mathbf{a}_s = \underline{\underline{\mathbf{A}}} \cdot \mathbf{a}_s,$$
 (552)

and multiply these equations from the right with \mathbf{a}_s and \mathbf{a}_r , respectively:

$$\omega_r^2 \mathbf{a}_s \cdot \underline{\underline{\mathbf{m}}} \cdot \mathbf{a}_r = \mathbf{a}_s \cdot \underline{\underline{\mathbf{A}}} \cdot \mathbf{a}_r$$

$$\omega_s^2 \mathbf{a}_r \cdot \underline{\underline{\mathbf{m}}} \cdot \mathbf{a}_s = \mathbf{a}_r \cdot \underline{\underline{\mathbf{A}}} \cdot \mathbf{a}_s.$$
(553)

²⁰Careful: this is not the usual orthogonality relation between two vectors, which would be $\mathbf{a}_r \cdot \mathbf{a}_s = \delta_{rs}$. The two relations differ if the masses m_{α} are not all the same.

Evaluating one of the matrix sandwiched between two vectors in components, and using the symmetry $A_{jk} = A_{kj}$,

$$\mathbf{a}_{s} \cdot \underline{\underline{\mathbf{A}}} \cdot \mathbf{a}_{r} = \sum_{j,k} a_{j,s} A_{jk} a_{k,r} = \sum_{j,k} a_{j,s} A_{kj} a_{k,r}$$
$$= \sum_{j,k} a_{k,r} A_{kj} a_{j,s} = \mathbf{a}_{r} \cdot \underline{\underline{\mathbf{A}}} \cdot \mathbf{a}_{s}, \qquad (554)$$

we see that the two right sides of (553) are the same. Similarly, due to $m_{kj} = m_{jk}$, the sandwich products $\mathbf{a}_s \cdot \underline{\mathbf{m}} \cdot \mathbf{a}_r$ and $\mathbf{a}_r \cdot \underline{\mathbf{m}} \cdot \mathbf{a}_s$ on the left sides of (553) are the same, so one can subtract the two equations and obtain

$$(\omega_s^2 - \omega_r^2) \mathbf{a}_r \cdot \underline{\mathbf{m}} \cdot \mathbf{a}_s = 0. \tag{555}$$

Assuming that the eigenfrequencies are not degenerate, the difference of its squares in the parenthesis does not vanish for $r \neq s$, and therefore, the sandwich product must vanish. This means that the two vectors obey the generalized orthogonality relation (553), which can be combined with the normalization (550) to

$$\mathbf{a}_r \cdot \underline{\mathbf{m}} \cdot \mathbf{a}_s = \delta_{rs} \,, \tag{556}$$

with the Kronecker symbol δ_{rs} .

The orthogonality of eigenvectors is one of the results of linear algebra; in fact, the whole search for the oscillation modes can be mapped to an eigenvector problem. To see this, we first recognize that the matrix $\underline{\mathbf{m}}$ can be inverted. For the simple case that the q_k are Cartesian coordinates, one can see from the definitions (536) and (538) of the matrix elements m_{jk} of $\underline{\mathbf{m}}$ that there are no off-diagonal elements, and the diagonal entries in $\underline{\mathbf{m}}$ are simply the masses corresponding to coordinate k:

$$m_{jk} = \delta_{jk} m_k \,. \tag{557}$$

Then, $\underline{\mathbf{m}}$ can be inverted²¹, with matrix elements of the inverse matrix $\underline{\mathbf{m}}^{-1}$

$$(\underline{\underline{\mathbf{m}}}^{-1})_{jk} = \delta_{jk} 1/m_k. \tag{558}$$

Therefore, we can multiply equation (545) from the left with $\underline{\mathbf{m}}^{-1}$, and obtain

$$(\underline{\underline{\mathbf{m}}}^{-1} \cdot \underline{\underline{\mathbf{A}}}) \cdot \mathbf{a} = \omega^2 \mathbf{a} \,, \tag{559}$$

which is the familiar eigenvector/eigenvalue equation from linear algebra for the matrix $\underline{\underline{\mathbf{m}}}^{-1} \cdot \underline{\underline{\mathbf{A}}}$, which is a $N \times N$ matrix if there are N degrees of freedom. There are N eigenvalues ω_r^2 , and the corresponding eigenvectors \mathbf{a}_r determine the oscillation modes. If the eigenvalues of a matrix are not degenerate, the corresponding eigenvectors are orthogonal. If there are degenerate eigenvalues, the

 $^{^{21} \}text{In fact, } \underline{\mathbf{m}}$ can always be inverted if there are no redundant coordinates.

subset of the corresponding eigenvectors is orthogonal to all other eigenvectors, and a linear combination of eigenvectors in that subspace can be found such that all eigenvectors are orthogonal. As the orthogonal vectors \mathbf{a}_r characterize the oscillation modes to an eigenfrequency ω_r , the modes are characterized by \mathbf{a}_r are also called *normal modes*.

10.2.2 Normal coordinates

In section 10.1.1 we introduced normal coordinates for the problem of two masses on an ad-hoc basis, and saw that the choice indeed decoupled the equations of motion. We can do this now for the general case, and introduce the connection between individual displacements u_k and normal coordinates η_r :

$$u_k(t) = \sum_r a_{k,r} \eta_r(t) , \qquad (560)$$

or in vectorial form

$$\mathbf{u} = \sum_{r} \mathbf{a}_r \eta_r(t) \,. \tag{561}$$

The transformation from the original coordinates u_k to normal coordinates can be accomplished by realizing that the eigenvectors \mathbf{a}_r are all orthogonal; when using normalization (556), one can multiply the relation (560) from the left with $\mathbf{a}_s \cdot \mathbf{m}$ to directly obtain the normal coordinate η_s :

$$\mathbf{a}_{s} \cdot \underline{\underline{\mathbf{m}}} \cdot \mathbf{u} = \mathbf{a}_{s} \cdot \underline{\underline{\mathbf{m}}} \cdot \sum_{r} \mathbf{a}_{r} \eta_{r}$$

$$= \sum_{r} \underbrace{\mathbf{a}_{s} \cdot \underline{\underline{\mathbf{m}}} \cdot \mathbf{a}_{r}}_{=\delta_{rs}} \eta_{r}$$

$$= \eta_{s}. \qquad (562)$$

This helps e.g. to express an initial condition given in \mathbf{u} in the normal coordinates. Since the coefficient matrices $\underline{\mathbf{m}}$ and $\underline{\mathbf{A}}$ do not depend on time, the velocities are

$$\dot{u}_k(t) = \sum_r a_{k,r} \dot{\eta}_r(t) \quad \text{or} \quad \dot{\mathbf{u}} = \sum_r \mathbf{a}_r \dot{\eta}_r(t) .$$
 (563)

The coupled Lagrange function in (540) can also be expressed in matrix form,

$$L = \frac{1}{2} \sum_{i,j} \left[m_{ik} \dot{u}_i \dot{u}_j - A_{ij} u_i u_j \right]$$
$$= \frac{1}{2} \left[\dot{\mathbf{u}} \cdot (\underline{\mathbf{m}} \cdot \dot{\mathbf{u}}) - \mathbf{u} \cdot \underline{\underline{\mathbf{A}}} \cdot \mathbf{u} \right], \tag{564}$$

assuming without loss of generality that $U_0 = 0$. Using expression (561) to make the transition to normal coordinates leads to

$$L = \frac{1}{2} \sum_{r,s} \dot{\eta}_r \dot{\eta}_s \underbrace{\mathbf{a}_r \cdot \underline{\mathbf{m}}}_{=\delta_{rs}} \cdot \mathbf{a}_s - \frac{1}{2} \sum_{r,s} \eta_r \eta_s \mathbf{a}_r \cdot \underline{\underline{\mathbf{A}}} \cdot \mathbf{s}_s, \qquad (565)$$

where the first sandwich product is just the orthogonality relation (556). For the second term, we use (545) for eigenvector \mathbf{a}_s ,

$$\underline{\mathbf{A}} \cdot \mathbf{a}_s = \omega_s^2 \underline{\mathbf{m}} \cdot \mathbf{a}_s \,, \tag{566}$$

and continue with the evaluation of the Lagrange function:

$$L = \frac{1}{2} \sum_{r} \dot{\eta}_{r}^{2} - \frac{1}{2} \sum_{r,s} \eta_{r} \eta_{s} \mathbf{a}_{r} \omega_{s}^{2} \underline{\mathbf{m}} \cdot \mathbf{a}_{s}$$

$$= \frac{1}{2} \sum_{r} \dot{\eta}_{r}^{2} - \frac{1}{2} \sum_{r,s} \eta_{r} \eta_{s} \omega_{s}^{2} \underbrace{\mathbf{a}_{r} \cdot \underline{\mathbf{m}} \cdot \mathbf{a}_{s}}_{=\delta_{rs}}$$

$$= \frac{1}{2} \sum_{r} \left[\dot{\eta}_{r}^{2} - \eta_{r}^{2} \omega_{r}^{2} \right]. \tag{567}$$

This is a sum of Lagrange functions for simple harmonic oscillators, which means that the motion in normal coordinates is completely decoupled. The corresponding equations of motion via Euler-Lagrange are

$$\frac{\partial L}{\partial \eta_r} - \frac{d}{dt} \frac{\partial L}{\partial \dot{\eta}_r} = -\omega_r^2 \eta_r - \frac{d}{dt} \dot{\eta}_r = 0$$
 (568)

or

$$\ddot{\eta}_r + \omega_r^2 \eta_r = 0 \qquad \text{for} \quad r = 1 \dots N \,, \tag{569}$$

which is a set of equations for N decoupled harmonic oscillators with the typical solutions

$$\eta_r(t) = \eta_r^+ e^{i\omega_r t} + \eta_r^- e^{-i\omega_r t}.$$
(570)

As before, the coefficients η_r^+ and η_r^- need to be chosen to meet initial conditions. To summarize, the strategy of solving a problem of small oscillations around the equilibrium of a coupled system of masses is as follows:

- Determine the mass matrix $\underline{\underline{\mathbf{m}}}$ either directly if the coordinates are the Cartesian coordinates, or via (536) and (538).
- Find the elastic coupling matrix $\underline{\mathbf{A}}$ according to (534).
- Find the eigenfrequencies ω_r and a set of corresponding normalized eigenvectors \mathbf{a}_r to the matrix $\mathbf{\underline{m}}^{-1} \cdot \mathbf{\underline{\Lambda}}$ for the normal modes of the system.
- Find a combination of amplitudes α_r and phase shifts δ_r for each eigenmode that satisfy the initial conditions via (548) and you are done!

In practice, this strategy can be followed for relatively small systems with not too many coordinates, because then the eigenvector search can be either done manually, or very efficient numerical methods can be used. The difficulty would be more in finding the elastic coupling matrix $\underline{\underline{\mathbf{A}}}$ if interaction between all masses take place. Examples for such problems are the vibrations that can occur in molecules.

10.3 Linear systems with next-neighbor couplings

We now come to a generalization of the problem of coupled masses presented in section 10.1 from 2 to N masses coupled to each other. The coupling should be restricted to close neighbors, as it is typical e.g. for lattice vibrations in a crystalline solid. However, the problem is much more general, because in various areas of physics one is restricted to such "local" interactions.

As the simplest example of such a problem, we consider again a linear chain of masses that can move in one direction, coupled by springs:

The system looks similar for all masses, i.e., all masses are the same and see a similar environment of neighbors and springs. The equation of motion is obtained in one of the usual ways, e.g. by considering the total force F_j acting on mass j:

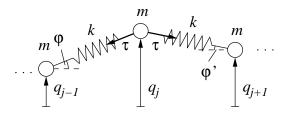
Force F_j is determined by position u_j of mass j, and those of its neighbors:

$$F_{j} = m\ddot{u}_{j} = -k(u_{j} - u_{j-1}) - k(u_{j} - u_{j+1})$$

$$= k(u_{j-1} + u_{j+1} - 2u_{j}).$$
(571)

Index j runs from 1 to N; we define $u_0 := 0$ and $u_{N+1} := 0$ to fulfill the boundary conditions at both ends of the chain in expression (571).

A very similar problem appears when we consider a transverse displacement of masses from an equilibrium position of a coupled string of masses. This approximates the situation of the string in a music instrument. The string should have a static tension force τ in equilibrium; the geometry of the problem is shown below:



The transverse restoring force for mass j is now given by

$$F_{j} = -\tau \sin \phi - \tau \sin \phi'$$

$$\approx -\tau (\tan \phi + \tan \phi')$$

$$= -\tau \left(\frac{q_{j} - q_{j-1}}{d} + \frac{q_{j} - q_{j+1}}{d}\right)$$

$$= \frac{\tau}{d} (q_{j-1} + q_{j+1} - 2q_{j}), \qquad (572)$$

leading to the same equation of motion as (571) with a different force coefficient:

$$m\ddot{q}_j = \frac{\tau}{d}(q_{j-1} + q_{j+1} - 2q_j). \tag{573}$$

Using the usual harmonic ansatz $u_j = a_j e^{i\omega t}$, we obtain the algebraic equation (545) for both the eigenfrequencies and the eigenvectors; in components:

$$-a_{j-1} + \lambda a_j - a_{j+1} = 0$$
 for $j = 1 \dots N$, with $\lambda = (2 - m\omega^2/k)$, (574)

or in matrix form with $\underline{\mathbf{D}} = \underline{\mathbf{A}} - \omega^2 \underline{\mathbf{m}}$:

$$\underline{\underline{\mathbf{D}}} \cdot \mathbf{a} = 0 \quad \text{or} \quad \begin{pmatrix} \lambda & -1 & 0 & 0 & \dots \\ -1 & \lambda & -1 & 0 & \dots \\ 0 & -1 & \lambda & -1 & \dots \\ & \vdots & \ddots & \end{pmatrix} \cdot \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix} = 0. \tag{575}$$

To satisfy this matrix equation, the characteristic equation must hold:

$$\det \mathbf{\underline{D}} = 0, \tag{576}$$

fixing the frequency ω of a solution. We verify this for two special cases. For N=1, the matrix $\underline{\mathbf{D}}$ reduces to the single value λ , and (576) simply becomes

$$\lambda = 0. (577)$$

From this, with the definition of λ in (574), we find

$$\omega = \sqrt{\frac{2k}{m}} \,. \tag{578}$$

Compared to the result (68) for the harmonic oscillator, the factor 2 here should not come as a surprise, because the we chose the boundary conditions such that the masses at the end are coupled to a wall with another spring on each side:

For N=2 we expect to reproduce the problem in section 10.1. We have

$$\underline{\underline{\mathbf{D}}} = \begin{pmatrix} \lambda & -1 \\ -1 & \lambda \end{pmatrix}, \quad \text{therefore} \quad \det \underline{\underline{\mathbf{D}}} = \lambda^2 - 1 = 0, \quad (579)$$

resulting in the solutions and corresponding eigenfrequencies seen in (513):

$$\lambda_{1,2} = \pm 1$$
, and $\omega_{1,2} = \sqrt{\frac{2 - \lambda_{1,2}}{m/k}} = \sqrt{\frac{2k \mp k}{m}}$. (580)

One could come up with a recursive expression for the characteristic equation for any N, but it is much more convenient to solve the problem differently.

10.3.1 Solution with the wave approach

In the algebraic equation system (574), the structure for all coefficients looks similar, with couplings only to next neighbors. We consider the ansatz

$$a_i = ae^{i(j\gamma - \delta)} \tag{581}$$

for the components of vector \mathbf{a} in (575), which is eigenvector to $\underline{\mathbf{m}}^{-1} \cdot \underline{\mathbf{A}}$. The coefficients a and δ should be real values, describing a common amplitude and phase for all components a_j , and γ a phase shift between neighboring components. The components $a_{j\pm 1}$ for the next neighbors are given by

$$a_{j\pm 1} = ae^{i([j\pm 1]\gamma - \delta)} = e^{\pm i\gamma}a_j,$$
 (582)

which helps to simplify (574):

$$-a_{j-1} - a_{j+1} + \lambda a_j = 0 \quad \to \quad (-e^{i\gamma} - e^{-i\gamma} + \lambda)a_j = 0 \quad \forall_{j=1...N}.$$
 (583)

Since the amplitude a_j is non-zero by construction (581), the parenthesis has to vanish, which leads to a condition between γ and λ :

$$2\cos\gamma = \lambda = 2 - \frac{m}{k}\omega^2 \tag{584}$$

or

$$\omega_r^2 = \frac{k}{m}(2 - 2\cos\gamma_r) = \frac{2k}{m}(1 - \cos\gamma_r) = \frac{4k}{m}\sin^2\frac{\gamma_r}{2} \quad \to \quad \omega_r = \sqrt{\frac{4k}{m}}\sin\frac{\gamma_r}{2}.$$
(585)

There, the index r indicates that we need to find r eigenfrequencies, and corresponding constants γ_r and δ_r . We now need to fix the values of γ_r and δ_r to meet the boundary conditions. As we are looking for real-valued displacements, we could have equally well chosen the real part of (582), at the cost of more complex expressions. We make this transition now:

$$a_{j,r} = a_r e^{i(j\gamma_r - \delta_r)} \quad \to \quad a_{j,r} = a_r \cos(j\gamma_r - \delta_r).$$
 (586)

The boundary condition at the left end (j=0) requires that $a_{0,r}=0$ or

$$0 = a_{0,r} = \cos(-\delta_r) \quad \Rightarrow \quad \delta_r = \frac{\pi}{2}, \quad \text{so} \quad a_{j,r} = a_r \sin(j\gamma_r). \quad (587)$$

The boundary condition on the right end of the chain requires

$$a_{N+1,r} = 0 \quad \Rightarrow \gamma_r(N+1) = s\pi \,, \quad s = 1, 2, 3, \dots$$
 (588)

Since we need N different solutions for ω_r , we simply choose s=r, so

$$\gamma_r = \frac{r \,\pi}{N+1} \,, \quad r = 1 \dots N \,. \tag{589}$$

This leads to eigenvector components

$$a_{j,r} = a_r \sin\left(j\frac{r\,\pi}{N+1}\right) \tag{590}$$

and with (585) to eigenfrequencies

$$\omega_r = \sqrt{\frac{4k}{m}} \sin \frac{r \,\pi}{2(N+1)} \,. \tag{591}$$

As in (560), we can express the individual deviations of the masses via normal coordinates η_r and the corresponding time dependence (570),

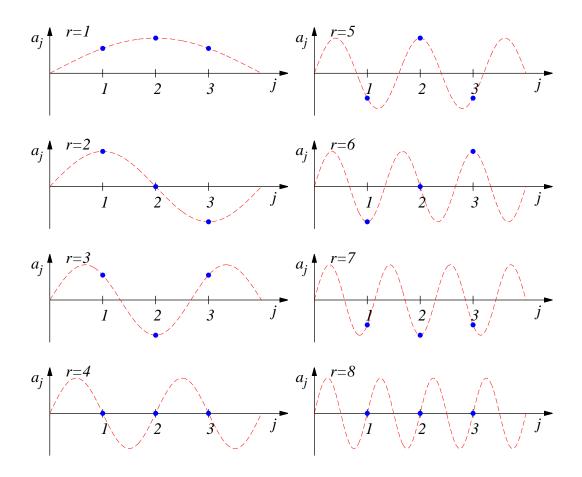
$$u_j(t) = \sum_r a_{j,r} \left[\eta_r^+ e^{i\omega_r t} + \eta_r^- e^{-i\omega_r t} \right],$$
 (592)

with adequate choices for the η_r^{\pm} to meet initial conditions if required.

10.3.2 Resulting mode structure

The mode structure contained in expression (590) resembles that of standing waves with different wavelengths; we visualize the different eigenvector components $a_{j,r}$ for the example with N=3 in the graph below. The eigenmodes for r=1...3 follow the pattern of standing waves, sampled at discrete points. The standing wave meets the boundary conditions at the auxiliary positions j=0 and j=N+1=4.

Modes for r=4 and r=8 do not lead to a meaningful oscillations, as all eigenvector components vanish. The modes corresponding to r=5,6,7 reproduce the modes structure corresponding to r=3,2,1, with an additional minus sign for all components. Hence, they do not constitute any new mode, and the description of modes with r=1,2,3 is indeed complete.



10.3.3 Dispersion relation

Since the amplitude distribution $a_{j,r}$ for the different modes r follow a standing wave pattern, we can use the wavelength of this wave to characterize the mode. For this, we assume that all masses spaced by the same distance d from their next neighbors. Then, the total length of the chain from endpoint to endpoint is L = (N+1)d. The wavelength of the fundamental mode (r=1) is then $\Lambda_1 = 2L$, and from (590) the wavelength of a higher order mode can be written as

$$\Lambda_r = \frac{2L}{r} \,. \tag{593}$$

One then can identify mass j also by its distance $x_j = jd$ from the left boundary corresponding to j = 0, and express the displacement u_j in that mode by

$$a_{j,r} = a_r \sin\left(j\frac{r\pi}{N+1}\right) = a_r \sin\left(\frac{(dj)r\pi}{L}\right)$$
$$= a_r \sin\left(x_j\frac{2L\pi}{\Lambda_r}\right) = a_r \sin\left(x_j\frac{2\pi}{\Lambda_r}\right) = a_r \sin\left(x_j\frac{2\pi}{\Lambda_r}\right). \tag{594}$$

Here, q_r is a wave number and indicates a spatial frequency:

$$q_r = \frac{2\pi}{\Lambda_r} = \frac{2\pi r}{2L} = \frac{r\pi}{(N+1)d}.$$
 (595)

Its maximal value is

$$q_{r,\text{max}} = q_N = \frac{\pi}{d} \frac{N}{N+1},$$
 (596)

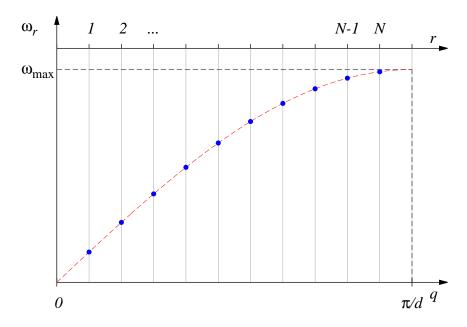
which converges to $q_{\text{max}} = \pi/d$ for large N. This is the typical situation e.g. for the motion of the atoms in a crystal, with lattice spacing d. There, the wave number q is a much better indicator for the mode as the integer mode index r because of the large number of atoms involved. The upper limit q_{max} corresponds to a minimal wavelength of $\Lambda_{\text{min}} = 2\pi/q_{\text{max}} = 2d$; a wavelength smaller than twice the lattice spacing d is not meaningful for a description of modes.

In the same way, the dependency of the eigenfrequencies ω_r in (591) from mode index r can be described by the wave number q:

$$\omega(q) = \sqrt{\frac{4k}{m}} \sin \frac{r\pi}{2(N+1)}$$

$$= \omega_{\text{max}} \sin \frac{qd}{2}, \quad \text{with} \quad \omega_{\text{max}} = \sqrt{\frac{4k}{m}}. \quad (597)$$

A function that relates the oscillation frequency of a mode with its wavenumber is called *dispersion relation* for a coupled system. The figure below shows the dispersion relation for a coupled linear chain of masses with N=10:



The maximal frequency ω_{max} corresponds to an oscillation mode where adjacent lattice sites oscillate in opposite direction; thus, the spring constant, compared to

the case of a single mass subject to two springs attached to a fixed wall, effectively doubles compared to the result (578).

The theory of coupled spring/mass systems is important in solid state physics; the problem above is only the simplest example of a lattice vibration in crystalline solids. It has to be extended to three dimensions, and typically, more complex crystal structures with more than one atom in a crystal unit cell need to be considered. But the basic treatment is the same as outlined in this section: oscillation modes are indexed by a wave number (or wave vector, in a three-dimensional case), and other parameters that indicate transverse or longitudinal displacements. As the frequencies of oscillation can be quite high in a solid, such oscillations need to be treated quantum mechanically, giving rise to "phonons" as quasi-particles corresponding to a particular mode index q. However, the whole dispersion relation of lattice vibrations is a purely classical mechanics problem.

10.4 Transition to a continuum

In the last section, we already replaced the particle index j by a position index x_j , and the discrete eigenmode index r by a wave number q. By increasing the number N of masses, while shrinking their distance d, but keeping the overall physical properties of the string, like its length L, total mass M and elastic properties fixed, we will arrive at a continuous distribution of masses and springs. This is a suitable description of solids, because it is often neither possible nor interesting to keep track of the position of all its constituting masses.

We first consider the basic variables of the problem. In the discrete case, these are the displacements u_j , which can be expressed by time-dependent normal coordinates η_r via (560), (594):

$$u_j(t) = \sum_r \eta_r(t) a_{j,r} = \sum_r \eta_r(t) \sin(x_j q_r).$$
 (598)

The η_r exhibit the simple harmonic oscillator dynamics (570) at frequency ω_r . Expression (598) has already a form to make the transition

$$u_j(t) \to u(x,t)$$
, (599)

to a function with a continuous position variable x. The time dependency of u for a given mode q still is a harmonic oscillation, but the $\omega(q)$ changes for $d \to 0$. For small d, we approximate the sinus in dispersion relation (597) for small angles:

$$\omega(q) = \sqrt{\frac{4k}{m}} \sin \frac{qd}{2}$$

$$\approx \sqrt{\frac{4k}{m}} \frac{qd}{2} = q \sqrt{\frac{d}{m}} \sqrt{kd}.$$
(600)

The result is written such that the first root is a ratio of distance over mass. If the global properties of the problems stay fixed, this ratio is the inverse of a

linear mass density ρ . The second root contains a product of a spring constant k and distance d, which also remains constant for the limit $d \to 0$: if a spring made out of a homogenous elastic material is cut in two pieces, an application of the same force to the short piece will lead to half the compression or extension of the original spring — to compress it to the same length, one would need to apply twice the force, i.e., the product of length d and spring constant k will not change. This product

$$K := kd \tag{601}$$

describes the stiffness of the material, and can be calculated from the elastic modulus or Young's modulus²² E of a material via $K = EA_0$ for a given cross section A_0 . Dispersion relation (600) then becomes

$$\omega(q) = q\sqrt{\frac{K}{\rho}}\,,\tag{602}$$

which is linear in q and has no upper limit for q or ω .

Similarly, a continuum relation for the transverse displacement for a string under a tensional force τ can be calculated: the equations of motion (571) for longitudinal, and (573) for a transverse displacement are essentially the same. All results for the longitudinal case can be transferred to the transverse case by replacing k with τ/d , changing the continuous dispersion relation (600) to

$$\omega(q) = q \sqrt{\frac{d}{m}} \sqrt{\frac{\tau}{d}} d = q \sqrt{\frac{\tau}{\rho}}.$$
 (603)

10.4.1 Coupled equations of motion in a continuum

Instead of transferring the results from a discrete problem to a continuum, one can also move from a discrete set of coupled equations of motion like (571) or (573) to a continuum description, and solve the problem directly. For this, we rewrite (571) to identify the continuum properties:

$$m\ddot{u}_j = k(u_{j+1} + u_{j-1} - 2u_j) \rightarrow \frac{m}{d}\ddot{u}_j = (kd)\left(\frac{u_{j+1} + u_{j-1} - 2u_j}{d^2}\right)$$
 (604)

The last parenthesis approximates the second derivative of u with respect to the position x_i . For $d \to 0$,

$$\frac{m}{d} \to \rho, \quad k d \to K, \quad \frac{u_{j+1} + u_{j-1} - 2u_j}{d^2} \to \frac{\partial^2 u(x)}{\partial x^2},$$
 (605)

so that the equation of motion (604) becomes

$$\rho \frac{\partial^2 u}{\partial t^2} = K \frac{\partial^2 u(x)}{\partial x^2} \qquad \text{or} \qquad \frac{\partial^2 u(x,t)}{\partial t^2} - \frac{K}{\rho} \frac{\partial^2 u(x,t)}{\partial x^2} = 0.$$
 (606)

 $^{^{22}\}mathrm{Named}$ after Thomas Young, 1773-1828, but discovered around 1727 by L. Euler.

This is a partial differential equation that mixes differentiations with respect to the different continuous variables x and t of the function u(x,t). The specific form of (606) is called wave equation, and has a particular set of solutions.

10.4.2 Solving the wave equation by separation of variables

One way of solving the wave equation is to assume a harmonic time dependency that is multiplied with some space-dependent part:

$$u(x,t) = v(x)e^{i\omega t}. (607)$$

Inserting this into the wave equation leads to

$$\left[-\omega^2 v(x) - \frac{K}{\rho} \frac{\partial^2 v(x)}{\partial x^2} \right] e^{i\omega t} = 0,$$
 (608)

where one can divide by the time-dependent oscillation, and end up with

$$\frac{\partial^2 v(x)}{\partial x^2} + q^2 v(x) = 0, \quad \text{with} \quad q^2 = \frac{\rho \omega^2}{K}. \tag{609}$$

This is an ordinary differential equation (or a simpler partial differential equation if more than one space dimension is involved), and is referred to as the $Helmholtz\ equation^{23}$. For one dimension x, it has the same structure as the equation of motion of a harmonic oscillator, which is consistent with finding sinusoidal solutions for the spatial structure of eigenmodes in (598). The q in expression (609) is exactly the wave number we used before, and we can directly extract the dispersion relation.

The observation of continuum solutions can actually help to motivate solutions for discrete variable cases; in section 10.3.1, the wave approach was presented without a reasoning, but the solution of a continuum problem really motivated the choice in (581).

10.4.3 Propagating solutions to the wave equation

Apart from solutions (598) we derived from a finite number of coupled masses, or could have gotten out of the Helmholtz equation (609), the wave equation (606) has other interesting solutions. We try the the ansatz

$$u(x,t) = w(x \pm vt), \qquad (610)$$

i.e., we replace the function of two variable by a function w of a single variable that is a combination of x and t. To check if this function can solve the wave

²³after Hermann von Helmholtz, 1821-1894

equation, we need derivatives of u with respect to t and x:

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial x} [w'(x \pm vt)] = w''(x \pm vt),
\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial t} [\pm v \, w'(x \pm vt)] = v^2 w''(x \pm vt),$$
(611)

where w'' indicates the second derivative of function w with respect to its parameter. Inserting those derivatives into the wave equation leads to

$$v^{2}w''(x \pm vt) - \frac{K}{\rho}w''(x \pm vt) = \left(v^{2} - \frac{K}{\rho}\right)w''(x \pm vt) = 0$$
 (612)

For $v^2 = K/\rho$, this equation can be fulfilled for *any* function w, as long as it is differentiable. This is a remarkable result: Any initial distribution u(x, t = 0) = w(x) is supported. Depending on the initial conditions, this distribution propagates either in positive or negative direction (or a combination of both) with a velocity

$$v = \sqrt{\frac{K}{\rho}}$$
, or $v = \sqrt{\frac{\tau}{\rho}}$ for transverse displacements. (613)

This velocity is therefore the *speed of sound* in a solid, as sound is the phenomenon of local displacements that propagate through material via elastic coupling.

10.4.4 Derivation of the wave equation via the Hamilton principle

While the transition from a discrete mass problem to a continuum in the last section leads to the correct wave equation of motion in an elastic one-dimensional continuum, the equation can also be derived via the Euler-Lagrange mechanism. The details are beyond the scope of this course, so we only cover this approach very briefly.

The basis for the Euler-Lagrange formalism is the knowledge of the total kinetic and total potential energy. We can make the transition from the total kinetic energy of the discrete chain to a continuum in a similar way as in the previous chapter:

$$T = \frac{1}{2} \sum_{j} m \dot{u}_{j}^{2} = \frac{1}{2} \frac{m}{d} \sum_{j} \dot{u}_{j}^{2} d.$$
 (614)

The ratio m/d is again the linear mass density ρ . The sum of over all velocities with the distance d can be replaced by an integral over the length of the string, leading for $d \to 0$ to the asymptotic expression for the total kinetic energy

$$T = \frac{1}{2}\rho \int_{0}^{L} \left(\frac{\partial u(x,t)}{\partial t}\right)^{2} dx.$$
 (615)

For the potential energy, we do a similar transition:

$$U = \frac{1}{2}k\sum_{j}(u_{j+1} - u_{j})^{2} = \frac{1}{2}(kd)\sum_{j}\left(\frac{u_{j+1} - u_{j}}{d^{2}}\right)^{2}d.$$
 (616)

The fraction in the sum (with the distance d) will become the partial derivative of the displacement with respect to x for $d \to 0$, and the sum will go over into an integral:

$$U = \frac{1}{2}K \int_{0}^{L} \left(\frac{\partial u(x,t)}{\partial x}\right)^{2} dx.$$
 (617)

Together with the kinetic energy T, this leads to a Lagrange function

$$L = T - U = \int_{0}^{L} \left[\frac{\rho}{2} \left(\frac{\partial u}{\partial t} \right)^{2} - \frac{K}{2} \left(\frac{\partial u}{\partial x} \right)^{2} \right] dx = \int_{0}^{L} \mathcal{L} \left(u, \frac{\partial u}{\partial t}, \frac{\partial u}{\partial x} \right) dx$$
 (618)

for the continuum, with a Lagrange density \mathcal{L} that depends on the function u(x,t), and its first partial derivatives with respect to x and t.

Without further proof, the equivalent to the Euler-Lagrange equation (194) for problems with two continuous parameters x and t is

$$\frac{\partial \mathcal{L}}{\partial u} - \frac{\partial}{\partial t} \left[\frac{\partial \mathcal{L}}{\partial \left(\frac{\partial u}{\partial t} \right)} \right] - \frac{\partial}{\partial x} \left[\frac{\partial \mathcal{L}}{\partial \left(\frac{\partial u}{\partial x} \right)} \right] = 0.$$
 (619)

The Lagrange density for the elastically coupled mass density in (618)

$$\mathcal{L}\left(u, \frac{\partial u}{\partial t}, \frac{\partial u}{\partial x}\right) = \frac{\rho}{2} \left(\frac{\partial u}{\partial t}\right)^2 - \frac{K}{2} \left(\frac{\partial u}{\partial x}\right)^2, \tag{620}$$

has partial derivatives

$$\frac{\partial \mathcal{L}}{\partial \left(\frac{\partial u}{\partial t}\right)} = \rho \, \frac{\partial u}{\partial t} \,, \quad \text{and} \quad \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial u}{\partial x}\right)} = -K \, \frac{\partial u}{\partial x} \,. \tag{621}$$

Inserting those into the Euler-Lagrange equation (619), and observing that \mathcal{L} does not explicitly depend on u (so $\partial \mathcal{L}/\partial u = 0$) leads to

$$-\frac{\partial}{\partial t} \left[\rho \frac{\partial u}{\partial t} \right] - \frac{\partial}{\partial x} \left[-K \frac{\partial u}{\partial x} \right] = -\rho \frac{\partial^2 u}{\partial t^2} + K \frac{\partial^2 u}{\partial x^2} = 0, \qquad (622)$$

which reproduces the wave equation (606).

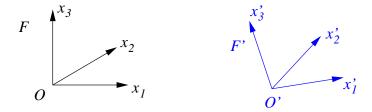
It should be stated that mechanical problems are usually never treated with this mechanism, since the formalism is way too complicated, and the respective partial differential equations for the displacement field u(x,t) can be obtained in a much simpler way. The method outlined above, however, is used in high energy physics, and when dealing with interactions that do not easily lead to field equations otherwise.

11 Non-inertial reference frames

So far, we have described mechanical problems only in inertial reference frames where Newton's first law holds, stating that a body not subject to a force remains in a state of uniform motion. However, there are important cases where inertial reference frames are inadequate or complicated. Notably, specifying the motion of bodies on the surface of the Earth is such an example. Because of the rotation of the Earth, Newton's laws (or equivalently, the equations of motion derived via the Euler-Lagrange formalism) do only hold approximately. In this section, we discuss a suitably modified version of Newton's second law in these systems.

11.1 Coordinate transformation

Consider two reference frames F and F' that are moving with respect to each other, and may also change their respective orientation over time:



The transformation at any instant can be separated in a translation between the two origins O and O', and a single rotation that adjusts the orientation of the coordinate systems with respect to each other (see section 1.4). If \mathbf{x} is a vector described by coordinates x_i in F, and by coordinates x_i' in F', i.e.

$$\mathbf{x} = \sum_{i=1}^{3} x_1 \mathbf{e}_1 + x_2 \mathbf{e}_2 + x_3 \mathbf{e}_3 = \sum_{i=1}^{3} x_1' \mathbf{e}'_1 + x_2' \mathbf{e}'_2 + x_3' \mathbf{e}'_3,$$
 (623)

then the two coordinate representations are connected via a rotation matrix \mathbf{R}

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \underline{\underline{\mathbf{R}}} \cdot \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} . \tag{624}$$

As seen in section 1.4, the rotation around the x_3 axis is e.g. represented by

$$\underline{\underline{\mathbf{R}}}_{3}(\phi) = \begin{pmatrix} \cos \phi & -\sin \phi & 0\\ \sin \phi & \cos \phi & 0\\ 0 & 0 & 1 \end{pmatrix}. \tag{625}$$

We then made the transition to infinitesimal rotations, e.g. for the x_3 axis

$$\underline{\underline{\mathbf{R}}}_{3}(\phi) \to \underline{\underline{\mathbf{R}}}_{3}(d\phi) = \underline{\underline{\mathbf{1}}} + \underline{\underline{\boldsymbol{\epsilon}}}_{3}(d\phi) = \underline{\underline{\mathbf{1}}} + \begin{pmatrix} 0 & -d\phi & 0 \\ d\phi & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{626}$$

with the unity matrix $\underline{\underline{1}}$. As shown in section 1.5, infinitesimal rotations around different axes can simply be added up, leading to the general infinitesimal correction matrix

$$\underline{\underline{\epsilon}}(d\phi_1, d\phi_2, d\phi_3) = \begin{pmatrix} 0 & -d\phi_3 & d\phi_2 \\ d\phi_3 & 0 & -d\phi_1 \\ -d\phi_2 & d\phi_1 & 0 \end{pmatrix}, \tag{627}$$

where the $d\phi_i$ describe infinitesimal rotations around coordinate axes *i*. If all infinitesimal rotations $d\phi_i$ are combined into a vector $d\boldsymbol{\phi} = (d\phi_1, d\phi_2, d\phi_3)$, the action of correction matrix $\underline{\boldsymbol{\epsilon}}$ can be expressed as a vector product:

$$\underline{\epsilon} \cdot \mathbf{x} = d\boldsymbol{\phi} \times \mathbf{x} \tag{628}$$

Therefore, we can rewrite the right side of (624) as

$$\underline{\underline{\mathbf{R}}} \cdot \mathbf{x} = (\underline{\underline{\mathbf{1}}} + \underline{\underline{\boldsymbol{\epsilon}}}) \cdot \mathbf{x} = \mathbf{x} + \underbrace{d\boldsymbol{\phi} \times \mathbf{x}}_{=:d\mathbf{x}}$$
 (629)

This means that for an infinitesimal rotation $d\phi$, the coordinate vector needs to be corrected by the infinitesimal amount $d\mathbf{x}$ to make the transition between two coordinate systems.

11.1.1 Transformation of time derivatives of vectors

Dividing the differential $d\mathbf{x}$ in (629) by an infinitesimal time dt leads to an expression for the temporal derivative of vector \mathbf{x} :

$$\frac{d\mathbf{x}}{dt} = \frac{d\boldsymbol{\phi}}{dt} \times \mathbf{x} = \boldsymbol{\omega} \times \mathbf{x}, \tag{630}$$

where ω is the instantaneous angular velocity. This expression reproduces the relation (30) between the instant velocity $\mathbf{v} = d\mathbf{r}/dt$ and the position \mathbf{r} introduced earlier, but holds for any vector \mathbf{x} , and allows evaluating the temporal derivative of a vector due to a rotation of the reference frame.

We now consider the temporal derivative of a vector \mathbf{x} expressed as a linear combination of base vectors $\mathbf{e'}_i$ of F',

$$\mathbf{x}(t) = \sum_{i} x_i'(t) \,\mathbf{e}'_i(t) \,. \tag{631}$$

Both the coefficients x'_i and the basis vectors \mathbf{e}'_i are time dependent, so

$$\frac{d\mathbf{x}}{dt}\Big|_{F} = \frac{d}{dt} \sum_{i} x_{i}' \mathbf{e'}_{i} = \sum_{i} (\dot{x}_{i}' \mathbf{e'}_{i} + x_{i}' \dot{\mathbf{e'}}_{i}) =: \frac{d\mathbf{x}}{dt}\Big|_{F'} + \sum_{i} x_{i}' \dot{\mathbf{e'}}_{i}$$
(632)

The index F indicates that the derivative is supposed to be taken in frame F, capturing both the time derivative of the coordinates x'_i and the base vectors

 $\mathbf{e'}_i$. The index F' in the temporal derivative of \mathbf{x} indicates that this is the derivative in system F': only the temporal derivatives of the coefficients x'_i are taken, multiplied with the base vectors $\mathbf{e'}_i$ that do not change in time in reference system F'. The second term contains temporal derivatives of $\mathbf{e'}_i$, as seen from reference frame F. For this, we can use (630):

$$\dot{\mathbf{e}'}_i = \frac{d\mathbf{e}'_i}{dt} = \boldsymbol{\omega} \times \mathbf{e}'_i, \tag{633}$$

With this, we can continue with the time derivative of \mathbf{x} :

$$\frac{d\mathbf{x}}{dt}\Big|_{F} = \frac{d\mathbf{x}}{dt}\Big|_{F'} + \sum_{i} x'_{i} (\boldsymbol{\omega} \times \mathbf{e'}_{i})$$

$$= \frac{d\mathbf{x}}{dt}\Big|_{F'} + \boldsymbol{\omega} \times \sum_{i} x'_{i} \mathbf{e'}_{i} = \frac{d\mathbf{x}}{dt}\Big|_{F'} + \boldsymbol{\omega} \times \mathbf{x}. \tag{634}$$

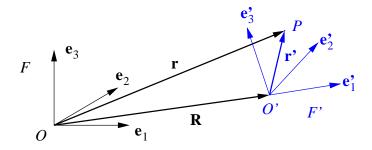
The temporal derivative of a vector \mathbf{x} as seen from reference frame F is therefore given by the temporal derivative of the vector as seen in reference frame F',

$$\left. \frac{d\mathbf{x}}{dt} \right|_{F'} = \sum_{i} \dot{x}_{i}' \, \mathbf{e'}_{i} \,, \tag{635}$$

corrected by a term that takes into account the time evolution of the base vectors $\mathbf{e'}_i$ of frame F' as seen from frame F.

11.1.2 Transformation of velocities and accelerations

We now consider the transformation of the characteristic vectors of a moving point P between two reference frames F and F'. The origin O' of F' should be displaced by a vector \mathbf{R} from the origin of F:



The position vector $\mathbf{r'}$ of point P with respect to origin O' can be expressed by vectors in system F:

$$\mathbf{r} = \mathbf{R} + \mathbf{r'}. \tag{636}$$

The displacement vector \mathbf{R} between the two reference frames may also change over time. Therefore, the velocity of P as seen from frame F is given by

$$\frac{d\mathbf{r}}{dt} = \frac{d\mathbf{R}}{dt} + \frac{d\mathbf{r'}}{dt}\Big|_{F}$$

$$= \frac{d\mathbf{R}}{dt} + \frac{d\mathbf{r'}}{dt}\Big|_{F'} + \boldsymbol{\omega} \times \mathbf{r'}, \qquad (637)$$

where the indices F and F' indicate the system with which respect a temporal derivative is taken. The above expression can be rewritten as

$$\mathbf{v} = \mathbf{V} + \mathbf{v}'_{F'} + \boldsymbol{\omega} \times \mathbf{r}', \tag{638}$$

where $\mathbf{V} = \dot{\mathbf{R}}$ is the velocity of origin O' in F, the velocity $\mathbf{v'}_{F'}$ of P is the one seen in system F' with respect to the origin O', angular velocity $\boldsymbol{\omega}$ captures the instantaneous change of orientation of the two coordinate systems.

To obtain the acceleration of point P, as seen from reference system F, we take another temporal derivative of (637):

$$\mathbf{a} = \frac{d\mathbf{V}}{dt} + \frac{d\mathbf{v'_{F'}}}{dt} \Big|_{F} + \left[\dot{\boldsymbol{\omega}} \times \mathbf{r'} + \boldsymbol{\omega} \times \frac{d\mathbf{r'}}{dt} \Big|_{F} \right]$$

$$= \ddot{\mathbf{R}} + \left(\frac{d\mathbf{v'_{F'}}}{dt} \Big|_{F'} + \boldsymbol{\omega} \times \mathbf{v'_{F'}} \right) + \left[\dot{\boldsymbol{\omega}} \times \mathbf{r'} + \boldsymbol{\omega} \times \left(\underbrace{\frac{d\mathbf{r'}}{dt} \Big|_{F'}}_{F'} + \boldsymbol{\omega} \times \mathbf{r'} \right) \right]$$

$$= \ddot{\mathbf{R}} + \mathbf{a'_{F'}} + 2\boldsymbol{\omega} \times \mathbf{v'_{F'}} + \dot{\boldsymbol{\omega}} \times \mathbf{r'} + \boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r'})$$
(639)

In the first line, only the time dependency of ω and $\mathbf{r'}$ was considered. From the first to the second line, the temporal derivatives of $\mathbf{v'}$ and $\mathbf{r'}$ were corrected for the rotation of the two reference frames with respect to each other. The newly introduced term $\mathbf{a'}_{F'}$ is the acceleration of P, as seen in reference frame F':

$$\mathbf{a}'_{F'} = \sum_{i} \ddot{r}'_{i} \mathbf{e}'_{i} \,. \tag{640}$$

11.2 Dynamics in non-inertial reference frames

So far, we only considered the kinematics of transformations between reference frames F and F'. We are not yet able to come up with a description of the dynamics of a system, as it was defined by Newton's second law.

To accomplish this, we now postulate that F is an inertial reference frame for which Newton's laws apply, while F' can be a non-inertial reference frame. The dynamics of a mass point m can then be described in the inertial reference frame F via Newton's second law (51):

$$\mathbf{F} = m \,\mathbf{a}\,,\tag{641}$$

where the force \mathbf{F} is a sum of all interactions with the environment or other masses, like gravitation, Coulomb interaction etc. Since there is also a meaningful acceleration vector $\mathbf{a}'_{F'}$ in the non-inertial reference frame F', we define an effective force \mathbf{F}_{eff} that allows writing down the equivalent to Newton's second law in the non-inertial reference frame:

$$\mathbf{F}_{\text{eff}} := m \, \mathbf{a}'_{F'} \,. \tag{642}$$

With the expression (639) for transforming the accelerations between F and F', we find

$$\mathbf{F}_{\text{eff}} = \mathbf{F} - m\ddot{\mathbf{R}} - m\dot{\boldsymbol{\omega}} \times \mathbf{r'} - 2m\boldsymbol{\omega} \times \mathbf{v'}_{F'} - m\boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r'})$$
 (643)

This means that in the non-inertial reference frame, the effective force \mathbf{F}_{eff} contains not only the "true" forces generated by interaction of masses, charges etc also seen in the inertial reference frame F, but also a number of so-called *inertial* forces that are a consequence of F' not being an inertial reference frame.

The first term results from an acceleration of the reference frame with respect to the inertial frame; this is the apparent force one observes in an accelerating elevator, or in an accelerating/decelerating vehicle. The second term is due to an angular acceleration, and has perhaps not an obvious presence in everyday life.

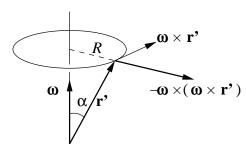
The third term is an apparent force that is proportional to the velocity $\mathbf{v}'_{F'}$ in the non-inertial reference frame F', and referred to as *Coriolis force*.

The last term in (643) is the *centrifugal force* that a body in reference frame F' feels that is proportional to the square of the angular velocity.

11.2.1 Centrifugal force

We first look at the geometry of the centrifugal force term in (643),

$$\mathbf{F}_{\text{centrif.}} = -m\boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r'}). \tag{644}$$



The orientation of the centrifugal force can be seen in the figure: For an origin O' of F' on the rotation axis, the vector $\boldsymbol{\omega} \times \mathbf{r'}$ is the velocity vector tangential to the trajectory of the point P. The resulting second vector product with the angular velocity $\boldsymbol{\omega}$ makes the centrifugal force pointing radially away from the rotation axis.

The modulus of the centrifugal force is given by

$$|\mathbf{F}_{\text{centrif.}}| = m \,\omega^2 \,|\mathbf{r'}| \sin \alpha = m \,\omega^2 R,$$
 (645)

where R is the shortest distance of P from the rotation axis, replicating the well-known expression for the centrifugal force.

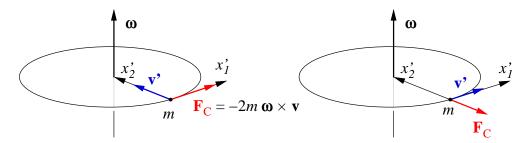
The centrifugal force is e.g. responsible for the deviation of the shape of the Earth from an ideal sphere; on the equator, the distance from the center of the earth is about 21.4km larger than on the poles due to the daily rotation. Furthermore, the direction of the local acceleration e.g. felt by a mass on a string does not point directly towards the center-of-mass of the earth, but must be corrected to take care of the centrifugal term.

11.2.2 Coriolis force

The Coriolis force term 24 in (643)

$$\mathbf{F}_{\text{Coriolis}} = -2m\boldsymbol{\omega} \times \mathbf{v'}_{F'} \tag{646}$$

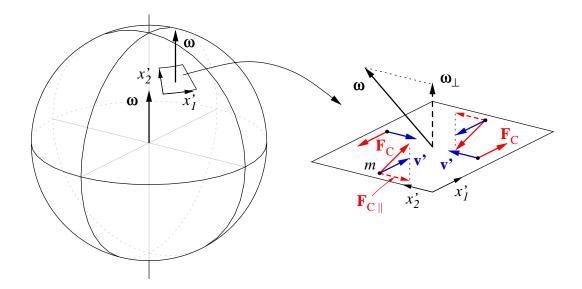
is only present if a body moves with respect to the moving reference system, i.e., $\mathbf{v'}_{F'} \neq 0$. The geometry of the Coriolis force can be easily seen for a mass point that moves with a velocity $\mathbf{v'}$ on a rotating platform:



In the left figure, the mass point is moving radially towards the center; in a coordinate system attached to the rotating platform, the velocity $\mathbf{v'}$ is parallel to the x_2' direction. The resulting Coriolis force according to (646) points in the x_1' direction. This can be understood in terms of an inertial effect: when moving radially in, the mass point has an angular momentum that would be too large for a new (static) position at a smaller radial distance. The mass point tries to retain its momentum, which appears as an accelerating force in the tangential direction in the rotating system. In the right figure, the velocity $\mathbf{v'}$ is along the x_1' direction, resulting in a Coriolis force pointing radially away from the rotation axis in the rotating frame. This can be interpreted as an additional centrifugal term, because with its additional tangential velocity, it appears to have a larger angular velocity than the rotating reference frame F'.

The Coriolis force has consequences on moving bodies on the surface of the Earth where observations are typically expressed in non-inertial coordinates (latitude and longitude) that are fixed to the rotating Earth. In a coordinate system (x'_1, x'_2) aligned with a tangential plane to the Earth, the angular velocity vector $\boldsymbol{\omega}$ in the northern hemisphere has a component $\boldsymbol{\omega}_{\perp}$ that points away from the surface of the earth.

 $^{^{24}}$ described by Gaspard-Gustave de Coriolis, 1792-1843; published in J. de l'Ecole royale polytechnique ${\bf 15},\,144-154\,\,(1835)$



If a mass moves in the tangential plane with a velocity $\mathbf{v'}$, the projection of the Coriolis force \mathbf{F}_C onto the tangential plane gives rise to a force that pulls the mass to the right side (with respect to its velocity, and seen when standing on the tangential plane). Consequently, air masses that move into a low pressure area on the northern hemisphere form a spiral that rotates counterclockwise around the low pressure area. However, only the component $\boldsymbol{\omega}_{\perp}$ of the angular velocity that is perpendicular to the tangential plane (x_1', x_2') contributes to an in-plane projection of the Coriolis force $\mathbf{F}_{C||}$.

On the equator, $\omega_{\perp}=0$ because the angular velocity vector $\boldsymbol{\omega}$ is parallel to the surface. For velocities $\mathbf{v'}$ tangential to the surface, the Coriolis force has therefore no component $\mathbf{F}_{C\parallel}$ in the tangential plane. On the southern hemisphere, the vertical component of the angular velocity vector points into the earth, leading to air moving into low pressure areas in clockwise spiraling motion.

The Coriolis force is also the basis of recent solid-state inertial sensors for rotation: in so-called *vibrating structure gyroscopes* or *MEMS gyroscopes*, an oscillating test mass feels the Coriolis force perpendicular to its oscillating motion if there is a rotation component perpendicular to the motion of the test mass. A similar effect seems to be used by some two-winged insects, which sense forces on so-called *halteres* vibrating with the wing frequency to determine their angular velocity and presumably stabilize their orientation in space.

12 Motion of rigid bodies

In the last section, we encountered a few effects related with the transformation between an inertial reference frame, and a rotating reference frame. However, we did not ask about the dynamics of a rotational motion. In this last section, we will address some of these aspects for so-called rigid bodies, i.e., an ensemble of mass points in a particular shape with a fixed relative position to each other.

12.1 Orientation of a rigid body in space - Euler angles

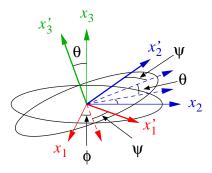
Several properties of rigid bodies are easy to describe in a coordinate system that is fixed to the rigid body. Such a coordinate system may not be an inertial reference frame, so we need to describe the relative orientation of the body coordinate system F' with respect to a fixed inertial system F. In section 1.4 we saw that this transformation can be expressed by a proper rotation, so we just need to parameterize this rotation. A common way to do this is to compose the rotation by three rotations around fixed axes such that a vector transforms as

$$\mathbf{x'} = \underline{\underline{\mathbf{R}}}_{3}(\psi) \cdot \underline{\underline{\mathbf{R}}}_{1}(\theta) \cdot \underline{\underline{\mathbf{R}}}_{3}(\phi) \cdot \mathbf{x}, \qquad (647)$$

with rotation matrices (see section 1.4)

$$\underline{\underline{\mathbf{R}}}_{3}(\phi) = \begin{pmatrix} \cos \phi & -\sin \phi & 0\\ \sin \phi & \cos \phi & 0\\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \underline{\underline{\mathbf{R}}}_{1}(\theta) = \begin{pmatrix} 1 & 0 & 0\\ 0 & \cos \theta & -\sin \theta\\ 0 & \sin \theta & \cos \theta \end{pmatrix}. \quad (648)$$

The angles ψ , θ , ϕ in (647) are referred to as *Euler angles*²⁵. The first rotation is around the x_3 axis, followed by a rotation around the x_1 axis, followed again by a rotation around the x_3 axis. Such a combination of rotations allows preparing any orientation of a rigid body in space. The figure below shows the orientation of the coordinate axes in the intermediate and final steps (for positive rotation angles ϕ , θ and ψ):



²⁵again after Leonhard Euler, 1707-1783

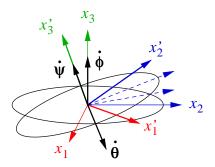
To work with the Euler angles in practice, the matrix multiplication (647) has to be directly carried out²⁶:

$$\underline{\mathbf{R}} = \underline{\mathbf{R}}_{3}(\psi) \cdot \underline{\mathbf{R}}_{1}(\theta) \cdot \underline{\mathbf{R}}_{3}(\phi) \qquad (649)$$

$$= \begin{pmatrix}
\cos \psi \cos \phi & -\cos \psi \sin \phi & \sin \psi \sin \theta \\
-\sin \psi \cos \theta \sin \phi & -\sin \psi \cos \theta \cos \phi & -\cos \psi \sin \theta \\
\sin \psi \cos \phi & -\sin \psi \sin \phi & -\cos \psi \sin \theta \\
+\cos \psi \cos \theta \sin \phi & +\sin \psi \cos \theta \cos \phi & \cos \theta
\end{pmatrix}.$$

12.1.1 Euler angles and angular velocity

In some situations, one can use the Euler angles as dynamic variables that describe the dynamics of the orientation of a body in an inertial reference frame. Then, the time derivatives of the Euler angles will become the generalized velocities. The changing angles can be represented by vectors $\dot{\phi}$, $\dot{\theta}$, and $\dot{\psi}$ pointing in the direction of the rotation axis as discussed in section 1.5:



Vector $\dot{\boldsymbol{\phi}}$ is aligned with the x_3 axis in the inertial system F, vector $\dot{\boldsymbol{\psi}}$ points into the direction of the x_3' axis in system F' attached to the rigid body, and $\dot{\boldsymbol{\theta}}$ points into the direction of the line of nodes where the two circles in the figure intersect. The instant values of $\dot{\boldsymbol{\phi}}$, $\dot{\boldsymbol{\theta}}$, and $\dot{\boldsymbol{\psi}}$ can be summed up to an angular velocity of the rigid body with respect to the inertial frame F. To be more useful in describing the dynamics later, we will describe this vector in system F' attached to the body.

The simplest case is that of the angular velocity associated to a change of Euler angle ψ , because it is already aligned with the basis vector 3 of F'. therefore, the components of $\dot{\psi}$ in F' are given by:

$$\dot{\psi}_1' = \dot{\psi}_2' = 0 \,, \quad \dot{\psi}_3' = \dot{\psi} \,, \tag{650}$$

²⁶To worsen this misery, not all texts use the same convention on how to count the Euler angles. Check carefully if you ever need them, or avoid them altogether when you can.

where $\dot{\psi}$ is simply the change of Euler angle ψ in time. Vector $\dot{\boldsymbol{\theta}}$ is parallel to the line of nodes, and therefore perpendicular to the x_3' axis; its components in F' are given by

$$\dot{\boldsymbol{\theta}}_{1}' = \dot{\boldsymbol{\theta}}\cos\psi, \quad \dot{\boldsymbol{\theta}}_{2}' = -\dot{\boldsymbol{\theta}}\sin\psi, \quad \dot{\boldsymbol{\theta}}_{3}' = 0. \tag{651}$$

Finally, the components of $\dot{\phi}$ in F' are given by

$$\dot{\phi}_1' = \dot{\phi}\sin\theta\sin\psi, \quad \dot{\phi}_2' = \dot{\phi}\sin\theta\cos\psi, \quad \dot{\phi}_3' = \dot{\phi}\cos\theta. \tag{652}$$

The total angular velocity vector ω due to a change of Euler angles in time is given by the sum of individual rotation vectors. In the reference system F' attached to the body, the components of ω are therefore given by

$$\boldsymbol{\omega} = \dot{\boldsymbol{\phi}} + \dot{\boldsymbol{\theta}} + \dot{\boldsymbol{\psi}} = \begin{pmatrix} \dot{\boldsymbol{\phi}} \sin \theta \sin \psi & + & \dot{\boldsymbol{\theta}} \cos \psi \\ \dot{\boldsymbol{\phi}} \sin \theta \cos \psi & - & \dot{\boldsymbol{\theta}} \sin \psi \\ \dot{\boldsymbol{\phi}} \cos \theta & + & \dot{\boldsymbol{\psi}} \end{pmatrix}. \tag{653}$$

12.1.2 Limitations of Euler angles to describe body orientations

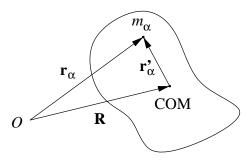
While every rotation of a rigid body with respect to an inertial system can be described by a set of Euler angles, its usefulness for practical problems is very limited. The problem is that not every rotation leads to a smooth evolution of the Euler angles. For example, a body reference system F' and the inertial reference system F are initially aligned, a rotation around axis x_2 would require the angle ϕ to jump to $\pi/2$ and ψ to $-\pi/2$, while θ follows the rotation. This problem is referred to as $gimbal\ lock$, and was a problem in early inertial guidance systems, among them one that occurred during the lunar landing mission of Apollo 11.

Therefore, other ways of representing the orientation of a body are often chosen. One can use the rotation matrix $\underline{\mathbf{R}}$ directly, but would have to store 9 entries. While this allows for fast vector transformations, this method has the disadvantage that it is numerically intensive to correct for numerical errors in matrices that are not exact rotations.

A method that requires four variables to store the orientation of a body, and avoids the gimbal lock problem as well as the re-normalization problem involves *quaternions*. They are an extension of the concept of complex numbers, with three roots of -1 and allow for an efficient calculation of concatenated rotations. Quaternions are beyond the scope of this course, but they form the basis of most orientation descriptions in current applications in navigation, robotics and computer graphics.

12.2 Inertia of a rigid body

A description of the dynamics of a rotating body requires an expression for its kinetic energy. We consider the rigid body to be made up by N masses m_{α} , with a fixed relative position with respect to each other. The positions of the masses forming the body are described in a coordinate system or reference frame F' fixed to the body, because there, the positions do not depend on the orientation of the body in space. The position \mathbf{r}_{α} of each particle is described by a center-of-mass position \mathbf{R} of the body with respect to some inertial reference frame F with origin O, and a distance vector $\mathbf{r'}_{\alpha}$ from the center-of-mass location:



By definition, the velocity of the individual masses making up the rigid body vanishes identically in the reference frame F' moving with the body:

$$\mathbf{v'}_{\alpha} = \left. \frac{d\mathbf{r'}_{\alpha}}{dt} \right|_{F'} \equiv 0. \tag{654}$$

Using (630), the velocity of mass m_{α} in inertial reference frame F is given by

$$\mathbf{v}_{\alpha} = \frac{d\mathbf{r}_{\alpha}}{dt}\Big|_{F} = \frac{d\mathbf{R}}{dt} + \frac{d\mathbf{r'}_{\alpha}}{dt}\Big|_{F} = \frac{d\mathbf{R}}{dt} + \underbrace{\frac{d\mathbf{r'}_{\alpha}}{dt}\Big|_{F'}}_{=0} + \boldsymbol{\omega} \times \mathbf{r'}_{\alpha}$$

$$= \mathbf{V} + \boldsymbol{\omega} \times \mathbf{r'}_{\alpha}, \qquad (655)$$

where V denotes the center-of-mass velocity of the body, and ω is the instantaneous rotation vector of the moving reference frame F' with respect to F.

12.2.1 Kinetic energy of a rigid body

With this, the kinetic energy of the body can be evaluated:

$$T = \frac{1}{2} \sum_{\alpha} m_{\alpha} \mathbf{v}_{\alpha}^{2} = \frac{1}{2} \sum_{\alpha} m_{\alpha} (\mathbf{V} + \boldsymbol{\omega} \times \mathbf{r'}_{\alpha})^{2}$$

$$= \frac{1}{2} \sum_{\alpha} m_{\alpha} \mathbf{V}^{2} + \sum_{\alpha} m_{\alpha} \mathbf{V} \cdot (\boldsymbol{\omega} \times \mathbf{R'}_{\alpha}) + \frac{1}{2} \sum_{\alpha} m_{\alpha} (\boldsymbol{\omega} \times \mathbf{r'}_{\alpha})^{2} \qquad (656)$$

$$= \frac{1}{2} \underbrace{\left(\sum_{\alpha} m_{\alpha}\right)}_{=M} \mathbf{V}^{2} + \mathbf{V} \cdot \left[\boldsymbol{\omega} \times \underbrace{\sum_{\alpha} m_{\alpha} \mathbf{r'}_{\alpha}}_{-M\mathbf{R'}}\right] + \frac{1}{2} \sum_{\alpha} m_{\alpha} (\boldsymbol{\omega} \times \mathbf{r'}_{\alpha})^{2},$$

where M is the total mass of the body. The second sum over masses contains the center-of-mass position $\mathbf{R'}$ in the body coordinate system F'. If the reference system F' is centered in the center-of-mass position of the body then $\mathbf{R'} = 0$, and the total kinetic energy can be written as

$$T = \frac{1}{2}M\mathbf{V}^2 + \frac{1}{2}\sum_{\alpha} m_{\alpha}(\boldsymbol{\omega} \times \mathbf{r'}_{\alpha})^2 =: T_{\text{trans}} + T_{\text{rot}}, \qquad (657)$$

i.e., the total kinetic energy is a sum of a translation part that only depends on the center-of-mass velocity V and the total mass M of the body, and a rotational energy $T_{\rm rot}$ that is independent from the center-of-mass motion.

The modulus of the vector product in the rotational energy can be converted to scalar products with the vector identity

$$(\mathbf{a} \times \mathbf{b})^2 = (\mathbf{a} \times \mathbf{b}) \cdot (\mathbf{a} \times \mathbf{b}) = (\mathbf{a} \cdot \mathbf{a})(\mathbf{b} \cdot \mathbf{b}) - (\mathbf{a} \cdot \mathbf{b})^2, \tag{658}$$

leading to the rotational energy

$$T_{\text{rot}} = \frac{1}{2} \sum_{\alpha} m_{\alpha} \left[\boldsymbol{\omega}^2 \mathbf{r'}_{\alpha}^2 - (\boldsymbol{\omega} \cdot \mathbf{r'}_{\alpha})^2 \right].$$
 (659)

We now evaluate the scalar products explicitly in Cartesian components:

$$T_{\text{rot}} = \frac{1}{2} \sum_{\alpha} \left[\left(\sum_{i=1}^{3} \omega_{i}^{2} \right) \left(\sum_{k=1}^{3} x'_{\alpha,k}^{2} \right) - \left(\sum_{i=1}^{3} \omega_{i} x'_{\alpha,i} \right) \left(\sum_{j=1}^{3} \omega_{j} x'_{\alpha,j} \right) \right]$$

$$= \sum_{\alpha} \sum_{i,j=1}^{3} m_{\alpha} \left[\omega_{i} \omega_{j} \delta_{ij} \left(\sum_{k=1}^{3} x'_{\alpha,k}^{2} \right) - \omega_{i} \omega_{j} x'_{\alpha,i} x'_{\alpha,j} \right]$$

$$= \frac{1}{2} \sum_{i,j=1}^{3} \omega_{i} \omega_{j} \left[\sum_{\alpha} m_{\alpha} \left(\delta_{ij} \left(\sum_{k=1}^{3} x'_{\alpha,k}^{2} \right) - x'_{\alpha,i} x'_{\alpha,j} \right) \right] = \frac{1}{2} \sum_{i,j=1}^{3} \omega_{i} \omega_{j} I_{ij}.$$

$$= I_{ij}$$

$$= I_{ij}$$

$$(660)$$

The total kinetic energy is therefore a bilinear function of the vector $\boldsymbol{\omega}$, with coefficients I_{ij} that only depend on the mass distribution in the rigid body. The coefficients I_{ij} can be written in matrix, and the kinetic energy becomes a "sandwich product" of a matrix between two vectors,

$$T_{\text{rot}} = \frac{1}{2} \boldsymbol{\omega} \cdot \underline{\underline{\mathbf{I}}} \cdot \boldsymbol{\omega}, \quad \text{with} \quad \underline{\underline{\mathbf{I}}} = \begin{pmatrix} I_{11} & I_{12} & I_{13} \\ I_{21} & I_{22} & I_{23} \\ I_{31} & I_{32} & I_{33} \end{pmatrix}.$$
 (661)

The object $\underline{\underline{I}}$ is referred to as the *inertia tensor* for the rigid body. A tensor associated with a physical property has slightly richer properties than a simple

matrix in the sense that it has well-defined transformation properties under similarity transformations. Before looking into this, we review the properties of the matrix entries of **I**:

$$\underline{\underline{I}} = \begin{pmatrix} \sum_{\alpha} m_{\alpha} (r'_{\alpha}^{2} - x'_{\alpha,1}^{2}) & -\sum_{\alpha} m_{\alpha} x'_{\alpha,1} x'_{\alpha,2} & -\sum_{\alpha} m_{\alpha} x'_{\alpha,1} x'_{\alpha,3} \\ -\sum_{\alpha} m_{\alpha} x'_{\alpha,2} x'_{\alpha,1} & \sum_{\alpha} m_{\alpha} (r'_{\alpha}^{2} - x'_{\alpha,2}^{2}) & -\sum_{\alpha} m_{\alpha} x'_{\alpha,2} x'_{\alpha,3} \\ -\sum_{\alpha} m_{\alpha} x'_{\alpha,3} x'_{\alpha,1} & -\sum_{\alpha} m_{\alpha} x'_{\alpha,3} x'_{\alpha,2} & \sum_{\alpha} m_{\alpha} (r'_{\alpha}^{2} - x'_{\alpha,3}^{2}) \end{pmatrix}.$$
(662)

The $x'_{\alpha,j}$ refer to the j-th component of the position of mass element α with respect to the center-of-mass of the body, and $r'^2_{\alpha} = x'^2_{\alpha,1} + x'^2_{\alpha,2} + x'^2_{\alpha,3}$ is the square of the distance of mass element α from the center-of-mass. The tensor entries are symmetric under index exchange:

$$I_{ij} = I_{ji} \,, \tag{663}$$

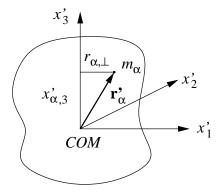
which reduces the independent tensor elements to three diagonal terms I_{11} , I_{22} , and I_{33} (referred to as moments of inertia), and three independent off-diagonal elements $I_{12} = I_{21}$, $I_{23} = I_{32}$, and $I_{13} = I_{31}$ (referred to as products of inertia).

12.2.2 Evaluation of the tensor elements

As shown in the figure below for the example of axis x_3 , the moments of inertia (diagonal elements of $\underline{\mathbf{I}}$) in (662) contain the difference

$$r'_{\alpha}^2 - x'_{\alpha,3}^2 = r'_{\alpha,\perp}^2,$$
 (664)

where r'_{\perp} is the distance to the rotation axis of mass element α . This reproduces the form for the moment of inertia known from elementary physics courses.



To evaluate the inertia tensor elements for continuous solids, the sum over all masses in (662) is replaced by an integral over the volume V of the body, and the masses m_{α} by a (possibly position-dependent) mass density $\rho(\mathbf{r}')$:

$$I_{ij} = \int_{V} d^3x' \rho(\mathbf{r'}) \left[\delta_{ij} \mathbf{r'}^2 - x_i' x_j' \right], \qquad (665)$$

with volume element d^3x' for the integration.

12.2.3 Angular momentum of a rigid body

From (123) in section 4.2, a rigid body has a total angular momentum

$$\mathbf{L} = \sum_{\alpha} \mathbf{r}_{\alpha} \times \mathbf{p}_{\alpha} = \mathbf{R} \times \mathbf{P} + \sum_{\alpha} \mathbf{r}_{\alpha}' \times \mathbf{p}_{\alpha}', \tag{666}$$

with center-of-mass position \mathbf{R} and total linear momentum \mathbf{P} . In the reference frame F' fixed to the body (with an origin at its center-of-mass), this simplifies to

$$\mathbf{L'} = \sum_{\alpha} \mathbf{r'}_{\alpha} \times \mathbf{p'}_{\alpha}. \tag{667}$$

The velocity $\mathbf{v'}_{\alpha}$ in $\mathbf{p'}_{\alpha}$ is given by (655) in an inertial reference frame F. It is referenced with respect to the center-of-mass of the body where $\mathbf{V'} = 0$, so

$$\mathbf{p'}_{\alpha} = m_{\alpha} \mathbf{v'}_{\alpha} = m_{\alpha} (\boldsymbol{\omega} \times \mathbf{r'}_{\alpha}). \tag{668}$$

With this, the total angular momentum (667) becomes

$$\mathbf{L'} = \sum_{\alpha} m_{\alpha} \mathbf{r'}_{\alpha} \times (\boldsymbol{\omega} \times \mathbf{r'}_{\alpha})$$

$$= \sum_{\alpha} m_{\alpha} \left[r'_{\alpha}^{2} \boldsymbol{\omega} - \mathbf{r'}_{\alpha} (\mathbf{r'}_{\alpha} \cdot \boldsymbol{\omega}) \right], \qquad (669)$$

where in the last step, we made use of the vector product identity

$$\mathbf{a} \times (\mathbf{b} \times \mathbf{a}) = (\mathbf{a} \cdot \mathbf{a})\mathbf{b} - \mathbf{a}(\mathbf{a} \cdot \mathbf{b}). \tag{670}$$

Expression (669) has two entries that are linear in ω ; to see this better, we look at the components of L':

$$L'_{i} = \sum_{\alpha} m_{\alpha} \left[r'_{\alpha}^{2} \omega_{i} - x'_{\alpha,i} \sum_{j} x'_{\alpha,j} \omega_{j} \right]$$

$$= \sum_{\alpha} m_{\alpha} \sum_{j} \left[\omega_{j} \delta_{ij} \sum_{k} x'_{\alpha,k}^{2} - x'_{\alpha,i} x'_{\alpha,j} \omega_{j} \right]$$

$$= \sum_{j} \left[\sum_{\alpha} m_{\alpha} \left(\delta_{ij} \sum_{k} x'_{\alpha,k}^{2} - x'_{\alpha,i} x'_{\alpha,j} \right) \right] = \sum_{j} I_{ij} \omega_{j}$$

$$= I_{ij}$$

$$(671)$$

with the same tensor components I_{ij} as in (660). The last expression is the result of a multiplication of vector $\boldsymbol{\omega}$ from the right side to tensor $\underline{\underline{\mathbf{I}}}$, so the total angular momentum can also be written as:

$$\mathbf{L'} = \underline{\underline{\mathbf{I}}} \cdot \boldsymbol{\omega} \,, \tag{672}$$

which is the rotation analog to the expression of the linear momentum $\mathbf{p} = m\mathbf{v}$. Inertia tensor $\underline{\mathbf{I}}$ therefore takes the role of the inertial object property for rotations, but it is not a simple scalar like the mass m. The total rotational energy (661) can be expressed as a scalar product using the angular momentum:

$$T_{\text{rot}} = \frac{1}{2} \boldsymbol{\omega} \cdot (\underline{\underline{\mathbf{I}}} \cdot \boldsymbol{\omega}) = \frac{1}{2} \boldsymbol{\omega} \cdot \underline{\mathbf{L'}}.$$
 (673)

12.2.4 Transformation properties of the inertia tensor

In section 1.4, we briefly mentioned that vectors and tensors as physical properties can be identified by their transformation properties under similarity transformations $\underline{\mathbf{M}}$. To see this, we take (672) and change the notation slightly, since the prime in $\mathbf{L'}$ just indicates that the angular momentum was to be taken with respect to a coordinate system originating in the COM of the rigid body. We now consider two versions of (672) in two coordinate systems F and F' that both originate in the COM of the rigid body:

$$\mathbf{L} = \underline{\mathbf{I}} \cdot \boldsymbol{\omega} \quad \text{and} \quad \mathbf{L'} = \underline{\mathbf{I'}} \cdot \boldsymbol{\omega'}.$$
 (674)

Both L and ω are vectors, so they obey the transformation rules

$$\mathbf{L'} = \underline{\mathbf{M}} \cdot \mathbf{L} \quad \text{and} \quad \boldsymbol{\omega'} = \underline{\mathbf{M}} \cdot \boldsymbol{\omega}$$
 (675)

with the same matrix $\underline{\mathbf{M}}$. Using this in (674) leads to

$$\underline{\mathbf{M}} \cdot \underline{\mathbf{I}} \cdot \boldsymbol{\omega} = \underline{\mathbf{M}} \cdot \mathbf{L} = \underline{\mathbf{I}'} = \underline{\mathbf{I}'} \cdot \boldsymbol{\omega'} = \underline{\mathbf{I}'} \cdot \underline{\mathbf{M}} \cdot \boldsymbol{\omega}. \tag{676}$$

This equality holds for all vectors $\boldsymbol{\omega}$, leading to the matrix identity

$$\underline{\underline{\mathbf{M}}} \cdot \underline{\underline{\mathbf{I}}} = \underline{\underline{\mathbf{I}'}} \cdot \underline{\underline{\mathbf{M}}} \tag{677}$$

or

$$\underline{\mathbf{I}'} = \underline{\mathbf{M}} \cdot \underline{\mathbf{I}} \cdot \underline{\mathbf{M}}^{-1} \tag{678}$$

which is the matrix version of the componentwise tensor transformation rule (43). This can be seen using

$$(\underline{\underline{\mathbf{M}}}^{-1})_{ij} = (\underline{\underline{\mathbf{M}}}^{T})_{ij} = (\underline{\underline{\mathbf{M}}})_{ji}$$
(679)

for similarity transformations $\underline{\mathbf{M}}$. Then,

$$I'_{ij} = (\underline{\underline{\mathbf{I}}}')_{ij} = (\underline{\underline{\mathbf{M}}} \cdot \underline{\underline{\mathbf{I}}} \cdot \underline{\underline{\mathbf{M}}}^{-1})_{ij}$$

$$= \sum_{kl} (\underline{\underline{\mathbf{M}}})_{ik} (\underline{\underline{\mathbf{I}}})_{kl} (\underline{\underline{\mathbf{M}}}^{-1})_{lj}$$

$$= \sum_{kl} m_{ik} I_{kl} m_{jl}, \qquad (680)$$

which is exactly the required transformation rule (43) for a tensor of rank 2. So the inertia tensor $\underline{\underline{I}}$ is a property of the rigid body, independent of the chosen coordinate system in which it is described.

12.2.5 Principal rotation axes of a rigid body

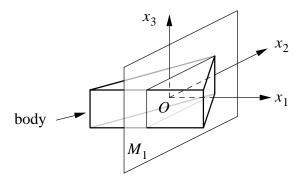
Relation (672) states that the inertia tensor $\underline{\underline{I}}$ linearly transforms the vector ω into another vector \underline{L} ; if ω and \underline{L} are parallel, they are eigenvectors of $\underline{\underline{I}}$. Each tensor $\underline{\underline{I}}$ has a set of three orthogonal eigenvectors $\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3$. In a coordinate system where base vectors \mathbf{e}_i are parallel to the eigenvectors \mathbf{i}_i , the inertia tensor takes a simple diagonal form:

$$\underline{\underline{\mathbf{I}}} = \begin{pmatrix} I_{11} & 0 & 0 \\ 0 & I_{22} & 0 \\ 0 & 0 & I_{33} \end{pmatrix} =: \begin{pmatrix} I_{1} & 0 & 0 \\ 0 & I_{2} & 0 \\ 0 & 0 & I_{3} \end{pmatrix}$$
(681)

The directions \mathbf{e}_i are called *principal rotation axes*, and for a rotation around them, the angular momentum \mathbf{L} is parallel to $\boldsymbol{\omega}$. The evaluation of the inertial tensor is particularly simple if the tensor $\underline{\underline{\mathbf{I}}}$ is evaluated in coordinates aligned with the principal rotation axes, as only three tensor elements need to be evaluated.

12.2.6 Relation between body symmetries and the inertia tensor

Evaluation of the inertial tensor is simple in the principal rotation axes, but it is not always obvious how these axes are oriented. Often the symmetry of the body gives an indication where they are. At the very least, symmetries can help to reduce the calculation effort. To see how this works, we first consider a body with a mirror symmetry. The example below has a mirror symmetry with respect to plane M_1 perpendicular to the x_1 axis:



The inertia tensor as a body property should therefore also be invariant under a mirror transformation, represented by a matrix $\underline{\mathbf{M}}_{1}$:

$$\underline{\underline{\mathbf{I}}} = \underline{\underline{\mathbf{I}'}} = \underline{\underline{\mathbf{M}}}_{1} \cdot \underline{\underline{\mathbf{I}}} \cdot \underline{\underline{\mathbf{M}}}_{1}^{-1} \quad \text{with} \quad \underline{\underline{\mathbf{M}}}_{1} = \underline{\underline{\mathbf{M}}}_{1}^{-1} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
(682)

The symmetry requirement is equivalent to

$$\underline{\underline{\underline{I}}} \cdot \underline{\underline{\underline{M}}}_{1} = \underline{\underline{\underline{M}}}_{1} \cdot \underline{\underline{\underline{I}}}, \tag{683}$$

which we now explicitly check by calculating the matrix products:

$$\underline{\underline{\mathbf{I}}} \cdot \underline{\underline{\mathbf{M}}} = \begin{pmatrix} -I_{11} & I_{12} & I_{13} \\ -I_{21} & I_{22} & I_{23} \\ -I_{31} & I_{32} & I_{33} \end{pmatrix} \quad \text{and} \quad \underline{\underline{\mathbf{M}}} \cdot \underline{\underline{\mathbf{I}}} = \begin{pmatrix} -I_{11} & -I_{12} & -I_{13} \\ I_{21} & I_{22} & I_{23} \\ I_{31} & I_{32} & I_{33} \end{pmatrix} . \quad (684)$$

Since both matrices need to be the same, we can immediately see by comparison that $I_{12} = I_{21} = I_{13} = I_{31} = 0$. The inertia tensor of a body with mirror symmetry in x_1 axis has therefore the form

$$\underline{\underline{\mathbf{I}}} = \begin{pmatrix} \cdot & 0 & 0 \\ 0 & \cdot & \cdot \\ 0 & \cdot & \cdot \end{pmatrix}, \tag{685}$$

where the dots indicate positions in the tensor that may not vanish. This matrix is block diagonal, so we already know that a vector parallel to the x_1 axis is an eigenvector of $\underline{\mathbf{I}}$, i.e., x_1 is a principal rotation axis of the rigid body. Similarly, one can show that the mirror symmetry in x_3 direction implies a form of the inertia tensor of

$$\underline{\underline{\mathbf{I}}} = \begin{pmatrix} \cdot & \cdot & 0 \\ \cdot & \cdot & 0 \\ 0 & 0 & \cdot \end{pmatrix}, \tag{686}$$

so the x_3 axis is also a principal rotation axis. Therefore, the x_2 axis is also a principal rotation axis, and tensor $\underline{\mathbf{I}}$ is diagonal in the shown coordinates. This method of identifying vanishing tensor entries due to symmetries requires very little effort, and simplifies the determination of tensor entries a lot.

The shown example has another symmetry: it is invariant under rotations around the x_3 axis by 120°. We consider the implications of this symmetry by looking at a rotation invariance under any rotation around the x_3 axis:

$$\underline{\underline{\mathbf{R}}}_{3}(\alpha) \cdot \underline{\underline{\mathbf{I}}} = \underline{\underline{\mathbf{I}}} \cdot \underline{\underline{\mathbf{R}}}_{3}(\alpha) \quad \text{with} \quad \underline{\underline{\mathbf{R}}}_{3}(\alpha) = \begin{pmatrix} c & -s & 0 \\ s & c & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{687}$$

where $c = \cos \alpha$ and $s = \sin \alpha$. Carrying out the two multiplications leads to

$$\underline{\underline{\mathbf{R}}}_{3}(\alpha) \cdot \underline{\underline{\mathbf{I}}} = \begin{pmatrix}
cI_{11} - sI_{21} & cI_{12} - sI_{22} & cI_{13} - sI_{23} \\
sI_{11} + cI_{21} & sI_{12} + cI_{22} & sI_{13} + cI_{23} \\
I_{31} & I_{32} & I_{33}
\end{pmatrix},$$

$$\underline{\underline{\mathbf{I}}} \cdot \underline{\underline{\mathbf{R}}}_{3}(\alpha) = \begin{pmatrix}
cI_{11} + sI_{12} & -sI_{11} + cI_{12} & I_{13} \\
cI_{21} + sI_{22} & -sI_{21} + cI_{22} & I_{23} \\
cI_{31} + sI_{32} & -sI_{31} + cI_{32} & I_{33}
\end{pmatrix}, (688)$$

which we now explore more carefully. By comparing the (1,1) entries in both matrices, we find

$$-sI_{21} = sI_{12} = sI_{21} (689)$$

because of the symmetry $I_{ij} = I_{ji}$ from (663). For rotation angles $\alpha \neq 0, \pi, ...$ where $s \neq 0$, this requires that

$$I_{12} = I_{21} = 0. (690)$$

This, by comparing the (1,2) components in (688), requires also

$$I_{11} = I_{22} \,. \tag{691}$$

Next, we compare the (3,1) entries in the products (688):

$$I_{31} = cI_{31} + sI_{32} \rightarrow \frac{I_{31}}{I_{32}} = \frac{s}{1 - c}$$
 (692)

for a non-vanishing I_{32} . The same procedure for the (3,2) entries gives

$$I_{32} = -sI_{31} + cI_{32} \rightarrow \frac{I_{31}}{I_{32}} = \frac{1-c}{-s}$$
 (693)

Both ratios have different signs, which only can be fulfilled if

$$I_{31} = I_{32} = I_{13} = I_{23} = 0. (694)$$

With these requirements, a tensor $\underline{\underline{I}}$ with a rotational symmetry other than 180° in x_3 direction has the simple form

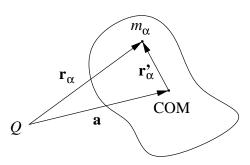
$$\underline{\underline{I}} = \begin{pmatrix} I_{11} & 0 & 0 \\ 0 & I_{11} & 0 \\ 0 & 0 & I_{33} \end{pmatrix}, \tag{695}$$

i.e., the axis of rotational symmetry is a principal rotation axis, and any axis in the x_1, x_2 plane is a principal rotation axis as well, with degenerate moments of inertia. A body with such properties is referred to as a *symmetric top*.

The exploration of symmetries to determine the number of independent entries in tensors goes far beyond the application to the tensor of inertia: In many areas of physics, symmetries e.g. in materials (due to their crystalline structure) imply if a physical property signified by a tensor takes a particular form, or is even present.

12.2.7 Inertia tensor for displaced rotation axes

In the derivation of the inertia tensor components, we assumed that the mass distribution is described in a coordinate system centered in the center-of-mass of the rigid body. However, often a rotation takes place around an axes not containing the center-of-mass, so it is interesting to calculate the inertia tensor elements with respect to a point Q that is displaced from the center-of-mass by a vector $-\mathbf{a}$:



To find the inertia tensor elements J_{ij} with respect to the new center Q, we recall expression (660) for the tensor elements in the center-of-mass system,

$$I_{ij} = \sum_{\alpha} m_{\alpha} \left[\delta_{ij} \left(\sum_{k=1}^{3} x'_{\alpha,k}^{2} \right) - x'_{\alpha,i} x'_{\alpha,j} \right], \qquad (696)$$

and evaluate the expression for displaced positions $\mathbf{r}_{\alpha} = \mathbf{r'}_{\alpha} + \mathbf{a}$ for the masses:

$$J_{ij} = \sum_{\alpha} m_{\alpha} \left[\delta_{ij} \left(\sum_{k=1}^{3} (x'_{\alpha,k} + a_{k})^{2} \right) - (x'_{\alpha,i} + a_{i})(x'_{\alpha,j} + a_{j}) \right]$$

$$= \underbrace{\sum_{\alpha} m_{\alpha} \left[\delta_{ij} \left(\sum_{k=1}^{3} x'_{\alpha,k}^{2} \right) - x'_{\alpha,i} x'_{\alpha,j} \right]}_{=I_{ij}}$$

$$+ \sum_{\alpha} m_{\alpha} \left[\delta_{ij} \left(\sum_{k=1}^{3} (a_{k}^{2} + 2x'_{\alpha,k} a_{k}) \right) - (a_{i}x'_{\alpha,j} + a_{j}x'_{\alpha,i} + a_{i}a_{j}) \right] (697)$$

In the second line, all terms that contain a single x'_{α} component appear in a sum over all α together with mass m_{α} . Since the $x'_{\alpha,k}$ are positions relative to the center-of-mass,

$$\sum_{\alpha} m_{\alpha} x'_{\alpha,k} = 0 \tag{698}$$

by definition. This simplifies the expression of the new tensor elements:

$$J_{ij} = I_{ij} + \sum_{\alpha} m_{\alpha} \left[\delta_{ij} \left(\sum_{k=1}^{3} a_{k}^{2} \right) - a_{i} a_{j} \right]$$
$$= I_{ij} + M[\delta_{ij} \mathbf{a}^{2} - a_{i} a_{j}], \qquad (699)$$

where M is the total mass of the rigid body. Thus, the inertia tensor $\underline{\underline{J}}$ with respect to a different rotation center Q than the center-of-mass is given by the sum of the inertia tensor $\underline{\underline{I}}$ of the body with respect to its center-of-mass and an inertia tensor by a single mass M, displaced by a vector $\underline{\mathbf{a}}$ from the rotation center. This is the so-called *parallel axis*— or *Huygens-Steiner* theorem²⁷.

 $^{^{\}rm 27}{\rm after}$ Christiaan Huygens, 1629-1695 and Jakob Steiner, 1796-1863

12.3 Equation of motion of a rotating rigid body

To describe the dynamics of a rotating body, we first choose a coordinate system F' fixed to the body that is aligned with the principal rotation axes. Then, the inertia tensor is diagonal, and the rotational energy (661) and angular momentum (672) are given by

$$T_{\text{rot}} = \frac{1}{2} \sum_{i=1}^{3} I_i \omega_i^2 \quad \text{and} \quad L_i = I_i \omega_i.$$
 (700)

The influence of external forces to the body is captured by a torque N acting on the body; we recall (129):

$$\frac{d\mathbf{L}}{dt} = \mathbf{N} \,. \tag{701}$$

This relation was derived in an inertial system, but it is most convenient to describe the dynamics of rotation in the coordinate system F' attached to the body. Therefore, we use the transformation rule (634) for time derivative of vectors between reference systems:

$$\mathbf{N} = \frac{d\mathbf{L}}{dt}\Big|_{F} = \frac{d\mathbf{L}}{dt}\Big|_{F'} + \boldsymbol{\omega} \times \mathbf{L}. \tag{702}$$

We now evaluate this equation for one component in the reference system F' attached to the body:

$$\frac{dL_1}{dt}\Big|_F = N_1 = \frac{dL_1}{dt}\Big|_{F'} + \omega_2 L_3 - \omega_3 L_2$$

$$= \frac{d(I_1\omega_1)}{dt}\Big|_{F'} + \omega_2 I_3\omega_3 - \omega_3 I_2\omega_2$$

$$= I_1\dot{\omega}_1 + \omega_3\omega_2 (I_3 - I_2). \tag{703}$$

The equations for the other components can be obtained by cyclic permutation of the indices:

$$N_2 = I_2 \dot{\omega}_2 + \omega_1 \omega_3 (I_1 - I_3)$$
 and
 $N_3 = I_3 \dot{\omega}_3 + \omega_2 \omega_1 (I_2 - I_1)$. (704)

These equation can be summarized in a compact notation with the totally anti-symmetric symbol ϵ_{ijk} :

$$(I_i - I_j)\omega_i\omega_j - \sum_k \epsilon_{ijk}(I_k\dot{\omega}_k - N_k) = 0.$$
 (705)

These equations are referred to as $Euler's^{28}$ equation of motion for the rigid body. They look relatively innocent, but what makes them hard to solve in practice is that the torque N must also be expressed in the reference system F' attached to the rotating body, which may require a knowledge of the instantaneous orientation in an external inertial reference frame.

²⁸same Leonhard Euler as before

12.4 Force-free rotation of a symmetric top

The solution of Euler's equation of motion (705) becomes relatively simple if there is no torque acting on the rotating body, and it is freely evolving. We start with the motion of a symmetric top with moments of inertia $I_1 = I_2 \neq I_3$. The equations of motion take the form

$$(I_{1} - I_{3})\omega_{2}\omega_{3} - I_{1}\dot{\omega}_{1} = 0$$

$$(I_{3} - I_{1})\omega_{3}\omega_{1} - I_{1}\dot{\omega}_{2} = 0$$

$$I_{3}\dot{\omega}_{3} = 0.$$
(706)

From the last equation, we find $\dot{\omega}_3 = 0$ or $\omega_3 = const.$, so the first two equations can be re-arranged:

$$\dot{\omega}_{1} = -\left(\frac{I_{3}-I_{1}}{I_{3}}\omega_{3}\right)\omega_{2} = -\Omega\omega_{2}$$

$$\dot{\omega}_{2} = \left(\frac{I_{3}-I_{1}}{I_{3}}\omega_{3}\right)\omega_{1} = \Omega\omega_{1}$$
(707)

with a constant

$$\Omega := \frac{I_3 - I_1}{I_1} \omega_3 \,. \tag{708}$$

This coupled set of equations can be easily solved by introducing a variable $\eta := \omega_1 + i\omega_2$, and adding the two equations (707) accordingly:

$$\dot{\omega}_1 + i\dot{\omega}_2 = -i\Omega(\omega_1 + i\omega_2) = 0 \quad \text{or}$$

$$\dot{\eta} - i\Omega\eta = 0.$$
 (709)

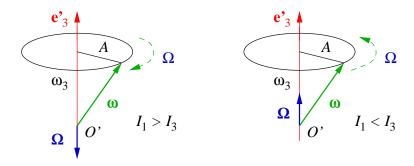
This simple linear equation of motion has a solution

$$\eta(t) = Ae^{i\Omega t} = A\cos\Omega t + iA\sin\Omega t, \qquad (710)$$

or, for the two components of the rotation vector,

$$\omega_1(t) = A \cos \Omega t
\omega_2(t) = A \sin \Omega t
\omega_3(t) = const.$$
(711)

We could have introduced a phase shift in the solution (710) to meet any initial condition, but that would not have substantially altered the solution for $\omega(t)$. The angular velocity vector ω (with modulus $|\omega| = \sqrt{\omega_3^2 + A^2}$ is precessing around the coordinate axis x_3' in the rotating reference frame F' with a precession angular frequency Ω from (708). Depending on the relative magnitude of I_1 and I_3 , the precession vector Ω (indicating the precession sense of ω) is either parallel or antiparallel to \mathbf{e}'_3 .



This still describes the dynamics of ω in the reference frame of the body. To transform this back to an inertial reference frame of an observer, we note that the force-free condition (and the fact that we have assumed no dissipation) requires that the rotational energy is constant:

$$T_{\rm rot} = \frac{1}{2} \boldsymbol{\omega} \cdot \mathbf{L} = const.$$
 (712)

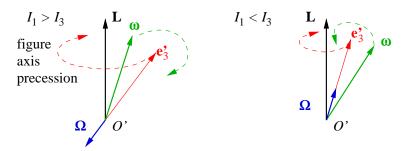
Furthermore, the total angular momentum of the system is conserved in an inertial reference frame F, i.e., the vector \mathbf{L} has both a constant modulus and direction. Energy conservation in the form of (712) requires that the projection of $\boldsymbol{\omega}$ onto \mathbf{L} and therefore the angle between them is constant as well. To understand the relative orientation of vectors \mathbf{L} , $\boldsymbol{\omega}$, and the principal axis of rotation $\mathbf{e'}_3$ (often referred to as the *figure axis* of the symmetric top because of the symmetry relation discussed earlier), we consider the vector product

$$\boldsymbol{\omega} \times \mathbf{e'}_3 = \omega_2 \mathbf{e'}_1 - \omega_2 \mathbf{e'}_2 \tag{713}$$

with the components ω_i in the rotating reference frame. This vector is perpendicular both to $\mathbf{e'}_3$ and $\boldsymbol{\omega}$. The scalar product

$$\mathbf{L} \cdot (\boldsymbol{\omega} \times \mathbf{e'}_3) = I_1 \omega_1 \omega_2 - I_2 \omega_2 \omega_1 = 0 \tag{714}$$

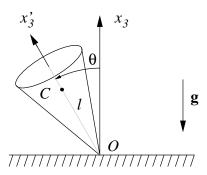
vanishes because $I_1 = I_2$ in the symmetric top. Therefore, **L** is perpendicular to $\boldsymbol{\omega} \times \mathbf{e'}_3$, which implies that **L**, $\boldsymbol{\omega}$ and $\mathbf{e'}_3$ are all in the same plane:



Depending on the ratio between I_1 and I_3 , the orientation of the three vectors is as shown in the figure; here, Ω denotes the direction of ω precessing around the figure axis $\mathbf{e'}_3$. In both cases, the angle between the figure axis and the angular momentum is constant, and the figure axis precesses around \mathbf{L} fixed in space.

12.5 Rotation of a heavy symmetric top

As an example of a more complex rotary motion, we consider the movement of a heavy symmetric top that is spinning around its figure axis, touching the ground at a single point O; the distance between the touching point O and the center-of-mass of the top C should be l:



In section 12.2.6 we saw that a rotationally symmetric top with a body coordinate system F' chosen to include the figure axis has a diagonal inertia tensor $\underline{\underline{I}}$ with two possibly different entries I_1 and I_3 .

The challenging part of this problem is the gravitational acceleration leading to a non-vanishing torque \mathbf{N} . This torque is well-defined in the inertial frame, but needs to be transformed into the body coordinate system F' to use the equations of motion (705) to describe the dynamics of the rotation vector. Furthermore, the rotation vector $\boldsymbol{\omega}$ would need to be integrated to obtain the orientation — a task that can not be accomplished as easily as for the force-free top.

This problem can be tackled if the Euler angles ϕ , θ and ψ describing the orientation of the top with respect to the inertial reference frame are taken as generalized coordinates for the problem. The equations of motion are then obtained with the standard Euler-Lagrange mechanism (206). For this, an expression for the kinetic energy T is needed; for the symmetric top, it is according to (661) and (695) given by

$$T_{\text{rot}} = \frac{1}{2} \sum_{i} I_{i} \omega_{i}' = \frac{1}{2} \left[I_{1} ({\omega'}_{1}^{2} + {\omega'}_{2}^{2}) + I_{3} {\omega'}_{3}^{2} \right].$$
 (715)

Note that in order to have only a rotational part of the kinetic energy, the inertia tensor elements need to be evaluated with respect to the origin O of F and F', and O is not the center-of-mass of the top. This is not a problem, because the figure is still rotationally symmetric with respect to x'_3 , hence $\underline{\underline{I}}$ is diagonal and has only two different entries I_1 , I_3 . Using the expression (653) for the angular velocity ω in the body coordinate system, one obtains a total kinetic energy as a function of the generalized coordinates and velocities:

$$T = \frac{1}{2} I_1 \left(\dot{\phi}^2 \sin^2 \theta + \dot{\theta}^2 \right) + \frac{1}{2} I_3 \left(\dot{\phi} \cos \theta + \dot{\psi} \right)^2.$$
 (716)

The potential energy is simply given by the total mass and the center-of-mass position,

$$U = Mgl\cos\theta\,, (717)$$

leading to the Lagrange function

$$L = T - U = \frac{1}{2} I_1 \left(\dot{\phi}^2 \sin^2 \theta + \dot{\theta}^2 \right) + \frac{1}{2} I_3 \left(\dot{\phi} \cos \theta + \dot{\psi} \right)^2 - Mgl \cos \theta.$$
 (718)

Immediately, one can identify ϕ and ψ as cyclic coordinates, leading to two constant corresponding generalized momenta

$$p_{\phi} = \frac{\partial L}{\partial \dot{\phi}} = \left(I_1 \sin^2 \theta + I_3 \cos^2 \theta \right) \dot{\phi} + I_3 \cos \theta \dot{\psi} = const., \quad (719)$$

$$p_{\psi} = \frac{\partial L}{\partial \dot{\psi}} = I_3 \left(\dot{\psi} + \dot{\phi} \cos \theta \right) = const.$$
 (720)

These quantities are angular momenta, and more specifically, projections of the total angular momentum **L** on the x_3 axis and x_3' axis, respectively. They can be used to obtain simple differential equations for the Euler angles ψ and ϕ :

$$\dot{\phi} = \frac{p_{\phi} - p_{\psi} \cos \theta}{I_1 \sin^2 \theta}, \tag{721}$$

$$\dot{\psi} = \frac{p_{\psi}}{I_3} - \frac{(p_{\phi} - p_{\psi}\cos\theta)\cos\theta}{I_1\sin^2\theta}.$$
 (722)

To solve the remaining problem, i.e., the time evolution of θ , we follow an approach of an *effective potential* similar to the central force problem in section 8.2. The system is conservative, so the total energy E should be conserved:

$$E = \frac{1}{2}I_1\left(\dot{\phi}^2\sin^2\theta + \dot{\theta}^2\right) + \underbrace{\frac{1}{2}I_3\omega'_3^2}_{=p_{\psi}^2/2I_3} + Mgl\cos\theta = const.$$
 (723)

By subtracting the (constant) kinetic energy term due to rotation around the figure axis from E one finds the relation

$$E - \frac{p_{\psi}^{2}}{2I_{3}} =: E' = \frac{1}{2}I_{1}\dot{\theta}^{2} + \frac{(p_{\phi} - p_{\psi}\cos\theta)^{2}}{2I_{1}\sin^{2}\theta} + Mgl\cos\theta$$
$$=: \frac{1}{2}I_{1}\dot{\theta}^{2} + V_{\text{eff}}(\theta), \qquad (724)$$

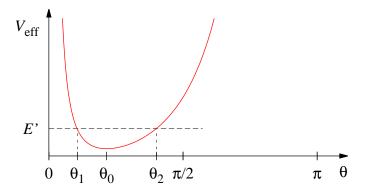
introducing an effective potential $V_{\text{eff}}(\theta)$ that only depends on the angular momentum constants p_{ψ} , p_{ϕ} and the coordinate θ .

Formally, one could integrate (724), and analogous to (328) in the central force problem obtain a function

$$t(\theta) = \int_{\theta_0}^{\theta} \frac{d\theta'}{\sqrt{\frac{2}{I_1}(E' - V_{\text{eff}}(\theta'))}},$$
 (725)

invert the result to obtain $\theta(t)$, and use (721/722) to obtain the solutions for the other two coordinates $\phi(t)$, $\psi(t)$. However, this can be reasonably done only numerically.

The type of motion can be characterized in a similar way as for the central force problem by looking at $V_{\text{eff}}(\theta)$:



For $p_{\phi} \neq p_{\psi}$, the effective potential limits the angle θ to the interval between 0 and π due to the $\sin^2 \theta$ term in the denominator of the effective potential in (724). The effective potential has a minimum at θ_0 , which can lead to a precession of the top with a constant angle θ_0 if the total excess energy E' is minimal. Otherwise, θ will oscillate between two extremal angles θ_1 and θ_2 . This oscillatory motion is referred to as *nutation*.

12.5.1 Precession of the heavy top without nutation

The minimum in the effective potential that leads to a motion with a constant angle θ_0 can be obtained by differentiating the effective potential. With the abbreviation

$$\beta := p_{\phi} - p_{\psi} \cos \theta \,, \tag{726}$$

that also appears in (719/720) for the other two Euler angles, the condition for a minimum of $v_{\rm eff}$ is

$$0 \stackrel{!}{=} \frac{\partial V_{\text{eff}}}{\partial \theta} \bigg|_{\theta=\theta_0} = \frac{\partial}{\partial \theta} \left[\frac{\beta^2}{2I_1} + Mgl \cos \theta \right]_{\theta=\theta_0}$$

$$= \frac{2\beta p_{\psi} \sin \theta_0 \sin^2 \theta_0 - \beta^2 2 \sin \theta_0 \cos \theta_0}{2I_1 \sin^4 \theta_0} - Mgl \sin \theta_0$$

$$= \frac{\beta p_{\psi} \sin^2 \theta_0 - \beta^2 \cos \theta_0 - Mgl I_1 \sin^4 \theta_0}{I_1 \sin^3 \theta_0}, \qquad (727)$$

or

$$\beta p_{\psi} \sin^2 \theta_0 - \beta^2 \cos \theta_0 - Mg l I_1 \sin^4 \theta_0 = 0.$$
 (728)

This equation has two solutions for β :

$$\beta_{\pm} = \frac{p_{\psi} \sin^2 \theta_0}{2 \cos \theta_0} \left[1 \pm \sqrt{1 - \frac{4MglI_1 \cos \theta_0}{p_{\psi}^2}} \right] . \tag{729}$$

For the solutions to be real, the argument of the root must be positive. Assuming that $\theta_0 < \pi/2$ (i.e., the top is above the surface), this requires

$$4MglI_1\cos\theta_0 < p_{\psi}^2 = I_3^2{\omega'}_3^2. \tag{730}$$

This condition imposes a minimum for the necessary angular momentum projection on the figure axis x'_3 , but allows for a range of possible angles θ_0 as long as the top spins fast enough. If the angular momentum p_{ψ} is much larger than this minimum, the square root in (729) can be approximated,

$$\sqrt{1 - \frac{4MglI_1\cos\theta_0}{p_{\psi}^2}} \approx 1 - \frac{2MglI_1\cos\theta_0}{p_{\psi}^2},$$
 (731)

leading to two approximate values for β of

$$\beta_{+} \approx \frac{p_{\psi} \sin^{2} \theta_{0}}{\cos \theta_{0}}, \quad \text{and} \quad \beta_{-} \approx \frac{MglI_{1} \sin^{2} \theta_{0}}{p_{\psi}}.$$
 (732)

For the change of the orientation of the figure axis in real space, i.e., the precession speed, we use (719), and find two values corresponding to the two values for β in (732):

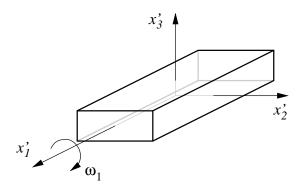
$$\dot{\phi}_{+} = \frac{\beta_{+}}{I_{1}\sin^{2}\theta_{0}} \approx \frac{p_{\psi}}{I_{1}\cos\theta_{0}} = \frac{I_{3}\omega_{3}'}{I_{1}\cos\theta_{0}},$$

$$\dot{\phi}_{-} = \frac{\beta_{-}}{I_{1}\sin^{2}\theta_{0}} \approx \frac{Mgl}{p_{\psi}} = \frac{Mgl}{I_{3}\omega_{3}'}.$$
(733)

The lower precession rate ϕ_{-} is apparently what is typically observed for this problem, leading to a faster and faster precession rate as a top slows down.

12.6 Stability of rotations of rigid bodies

Even the very simple case of a force-free rotation of a complex object around its principal rotation axes is not as simple as it appears; we consider a rigid body with a coordinate system aligned to its principal rotation axes, assuming $I_3 > I_2 > I_1$:



If the body rotates approximately but not exactly around the x'_1 axis, the angular velocity vector can be written as

$$\boldsymbol{\omega} = \omega_1 \mathbf{e'}_1 + \lambda \mathbf{e'}_2 + \mu \mathbf{e'}_3$$
, with $\lambda, \mu \ll \omega_1$. (734)

Euler's equations of motion for the force-free rotating body (705) allow determining the time-dependence of the coefficients ω_1 , λ and μ :

$$(I_2 - I_3)\lambda \mu - I_1 \dot{\omega}_1 = 0, (735)$$

$$(I_3 - I_1)\mu\omega_1 - I_2\dot{\lambda} = 0, (736)$$

$$(I_1 - I_2)\lambda\omega_1 - I_3\dot{\mu} = 0. (737)$$

Since we start out with small perturbations of the rotation vector from the principal axis, we can approximate the product $\lambda\mu$ in (735) initially by 0, so the angular velocity ω_1 remains constant over time:

$$-I_1\dot{\omega}_1 = 0 \quad \to \quad \omega_1 = const. \tag{738}$$

The other two equations lead to a coupled system of differential equations,

$$\dot{\lambda} = \frac{I_3 - I_1}{I_2} \omega_1 \mu \,, \quad \dot{\mu} = \frac{I_1 - I_2}{I_3} \omega_1 \lambda \,.$$
 (739)

We can not use the same trick as for the force-free symmetric top in section 12.4, because the coupling constant is not the same. Instead, we can chain the equations, effectively eliminating the variable μ :

$$\ddot{\lambda} = \frac{I_3 - I_1}{I_2} \omega_1 \dot{\mu} = \frac{I_3 - I_1}{I_2} \frac{I_1 - I_2}{I_3} \omega_1^2 \lambda \tag{740}$$

or

$$\ddot{\lambda} + \Omega_1^2 \lambda = 0 \quad \text{with} \quad \Omega_1 := \omega_1 \sqrt{\frac{(I_1 - I_3)}{I_2} \frac{(I_1 - I_2)}{I_3}}.$$
 (741)

This second order linear differential equation for $\lambda(t)$ has the familiar solution

$$\lambda(t) = Ae^{i\Omega_1 t} + Be^{-i\Omega_1 t}. \tag{742}$$

For $I_1 < I_3$ and $I_1 < I_2$, as postulated initially, the angular frequency Ω_1 is real, resulting in an oscillatory evolution of the rotation components along axes x_2' and x_3' with a fixed amplitude. This means that small deviations of ω from the principal axis x_1' remain small.

The situation changes if the rotation takes place around axis x'_2 ; by cyclic permutation from the expression in (741) one obtains

$$\Omega_2 = \omega_2 \sqrt{\frac{(I_2 - I_1)}{I_3} \frac{(I_2 - I_3)}{I_1}}.$$
 (743)

This time, the expression in the square root becomes negative, resulting in an imaginary Ω_2 and therefore an exponentially growing contribution in the equivalent solution to (742). Thus, a small deviation of the angular velocity vector from axis x_2 does not lead to a stable rotation. For a rotation around axis x_3' with the largest moment of inertia, one obtains

$$\Omega_3 = \omega_3 \sqrt{\frac{(I_3 - I_2)}{I_1} \frac{(I_3 - I_1)}{I_2}}, \tag{744}$$

which is real-valued again, resulting in a stability of small perturbations of the rotation axis alignment with x'_3 , similar to the rotations around x'_1 . In summary, rotations around the axis with the largest and with the smallest moment of inertia are stable, a rotation around the third axis is *unstable* for a rigid body with three different principal moments of inertia.

12.6.1 Symmetric top

For a symmetric top, with $I_1 = I_2$ a rotation around axis x'_1 can be treated similarly, but the equation of motion for μ in (739) becomes simpler:

$$\dot{\mu} = 0 \quad \rightarrow \quad \mu = const. \tag{745}$$

consequently, the equation for λ leads to a non-oscillating solution for the perturbation component,

$$\dot{\lambda} = \frac{I_3 - I_1}{I_2} \omega_1 \mu = const. \quad \to \lambda(t) = At + B, \tag{746}$$

which is not limited over time. Thus, the rotation of a symmetric top around an axis other than the figure axis is unstable, and only the rotation around the figure axis x_3' is stable.