

Theoretical Mechanics

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Axel Maas

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Chapter 1

Introduction

Theoretical mechanics is, in a sense, a somewhat ancient topic. Essentially completely formulated in its modern form in the 19th century, it has matured into a mathematically consistent and closed theory. Even the advent of special relativity only required a minor modification of the underlying vector spaces in the mathematical formulation, and could therefore be technically easily accommodated. Of course, the interpretational impact has been of much more significance.

The natural question is therefore why it is necessary to discuss it then at all. The answer to this is that all modern models in physics draw from the conceptual structure of classical mechanics. General relativity introduced again modifications of the arena. Quantum physics modified the nature of coordinates themselves. But the basic formulation tools of theoretical mechanics, especially the Lagrangian formulation of chapter 4 and the Hamiltonian formulation of chapter 5, are still mathematical cornerstones of these theories. It is not the concept which changed, merely the entities on which it is applied, at least from a mathematical point of view. Of course, again the shifts in physical interpretation had a much larger impact.

Thus, theoretical mechanics remains both mathematical and in terms of conception still a cornerstone of even the most modern areas of physics. Understanding theoretical mechanics in these formulations is therefore forming the foundation on which these are build.

However, these formulation as Lagrangian and Hamiltonian mechanics in chapters 4 and 5, as powerful as they are, are very dissimilar from the usual concept of Newton's law, even if they embody the same physics. In fact, at first sight it is far from obvious that reformulating mechanics mathematically in this way could be anything but obscuring. It is only when making the transition to quantum physics and general relativity that their conceptual importance becomes really evident.

If one would embark on either topic without first going through the mathematical reformulation of mechanics would require to cope at the same time with quite different mathematical and conceptual problems. Classical mechanics, and to some extent special relativity, are therefore role models for the future.

To provide a smooth transition from the experimental view on mechanics to the theoretical formulation, the first step will be to give a more theoretical perspective on Newtonian mechanics in chapter 2, sometimes also called analytical mechanics. In this way, the theoretical approach to physics problems is best outlined, as here the subject of study, ordinary Newtonian mechanics, is already well acquainted from experimental physics, so that one can concentrated on the more abstract theoretical formulation.

The next step is then to introduce the ideas of special relativity in chapter 3. This allows to introduce the central concepts later then not only for Newtonian mechanics, but already in parallel for the case of special relativity.

The first version of reformulation of mechanics is then Lagrangian mechanics in chapter 4. There are two versions of this, both having their own advantages. Lagrange's equations of the first kind in section 4.7 are extremely useful when it comes to problems in applications of classical mechanics. However, some of the concepts will also be relevant in statistical physics, the microscopical explanation of thermodynamics. Lagrange's equation of the second kind in section 4.4 are the natural way to formulate problems embodying special relativity and quantum physics simultaneously, which is the arena of particle physics. Afterwards, another reformulation is given in terms of Hamilton's mechanics in chapter 5. This reformulation is especially useful for non-relativistic quantum physics. It may appear odd at first sight that this more special case, as it does not lend itself so easily to special relativity, is treated after the more general case. But this formulation is actually easier to understand from the Lagrangian formulation as then from starting outright towards it. Finally, these methods will then be used to treat some special topics in classical mechanics in chapter 6.

There are numerous textbooks on the topic of theoretical mechanics, from the rather hands-on treatments of the books in the two classic series on theoretical physics of Noltting and Greiner, up to the modern treatment of Bartelmann et al., as well as the more abstract classical treaty of Goldstein. The number of books is essentially legion. Any real recommendation is too much depending on personal taste and difficulty preference, and it is therefore highly recommendable to choose accordingly to one's own taste. This lecture does not follow any of these books particularly, but draws instead from many sources.

Chapter 2

Newtonian mechanics

The aim of this first chapter is not necessarily to introduce new physics or new physics concepts. After all, Newtonian physics is familiar from experimental physics. The main aim here is to provide a new perspective on it. So far, the exposure to physics was mainly by means of understanding experiments. The theoretical approach is somewhat different. The basic idea is to start from a set of fixed rules, e. g. Newton's laws. The next step is then to derive consequences of these laws, e. g. the movement of the earth around the sun. Comparison between these derived results and experiments then decides whether the basis of the derivation is actually useful to describe experiments or not.

Of course, the aim of this exercise is to end up with the minimal basis to describe all experimental results. This is often considered as the basic laws of nature. Whether they are indeed ingrained in reality in some way is a highly non-trivial questions, and not (yet?) resolved. However, to even pose this question requires to be able to connect some limited set of basic principles with experiments. This is the task of theoretical physics. This also includes, of course, to identify this basic set. The resulting basis is called a (standard) model or a theory, while the constructions still awaiting experimental tests are usual considered as hypothesis. There are fine distinctions between these names which, however, play no role in this lecture, nor actually in the day-to-day research.

Note, however, that any experiment can at most falsify a theory. It can never prove it to be correct. Thus, any theory or model can only be considered to be an adequate description for the time being. Though often theories are refuted entirely based on contradiction to experiment, there are some cases where they do contradict experiments, but are not really refuted. In this case, the theory turns out to be the limit of a more general theory in a particular case. E. g., Newtonian mechanics will be the limit of special relativity for small speeds. Only when experiments become sensitive enough they can detect this situation.

A special limit theory is by no means useless. When building a bridge, nobody will do

the statics using special relativity, but ordinary Newtonian mechanics. Thus such a limit theory, more often called an effective theory, is by no means useless. Quite often the more general theory is of less practical use.

2.1 Kinematics

Before starting with physics, sometimes also called dynamics, it is useful to first consider the description of (point) particles, the central entities of mechanics. This is a pure description, and there is no answers to why a particle behaves in a certain way. To separate this from the actual reasons of their movement this is often called kinematics.

The starting point for the description of a particle is the path it follows during an interval of time. In general, this path is described by a vector-valued function $\vec{r}(t)$ in a vector space. This vector space describes the position of the particle in space, while time acts as a parameter to identify the position of the particle along its path, which is also called a trajectory.

In the following, the vector space will be the ordinary \mathbb{R}^3 , sometimes also \mathbb{R}^2 or even \mathbb{R}^1 , equipped with the usual scalar product and norms to obtain a Hilbert space.

The speed \vec{v} of a particle is defined to be

$$\vec{v}(t) = \frac{d\vec{r}(t)}{dt},$$

i. e. the rate of change of the position of the particle along its path. Usually, the path of particles will be infinitely often differentiable, so this is a well-defined quantity. In mechanics, however, usually only the second differential,

$$\vec{a}(t) = \frac{d\vec{v}(t)}{dt} = \frac{d^2\vec{r}(t)}{dt^2}$$

plays also an important role. The others may appear, but are not central quantities.

With these definitions, the behavior of a particle can be described (though not explained). If there are multiple particles, their paths will be indexed.

Given the acceleration, it is possible to obtain the path by twofold integration,

$$\vec{r}(t) = \vec{r}(t_0) + \vec{v}(t_0)(t - t_0) + \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' a(t''),$$

where the quantities $r(t_0)$ and $v(t_0)$ are the position and speed at time t_0 , the initial conditions. Similarly, if the speed or higher derivatives are given, the path can be obtained by a single or even more integrations.

2.2 Newton's laws

2.2.1 Preliminaries

While the previous section provided the tools to describe the movement of a particle, it did not give any reason how, e. g., the acceleration comes about. This is the question of dynamics.

As alluded to earlier, the first step in theoretical physics is to define a basis, i. e. a set of laws which describe the dynamics. In analogy to mathematics, these are sometimes also called axioms, but more often nowadays just as the model, given the insight that all models have their limits.

Classical mechanics is the theory which is based upon Newton's laws. They were found in a long sequence of interplay between theory and experiment. This history of physics will not be traced out here, but it should be noted that the formulation of the model is by no means a trivial exercise, and all laws of physics have been created based on a multitude of experimental insights, no matter how many spectacular things later were predicted by them.

2.2.2 The first law

To formulate Newton's laws, it is necessary to introduce a few more concepts. The first is to define a force as the origin of dynamics. I. e., without forces, the particle will not change its kinematics. To give this statement a more precise meaning requires the notion of an inertial system.

The first law of Newton is that if no forces act on a particle then there exists a co-ordinate system in which its acceleration and all higher derivatives of its path vanish identically, and thus the particle either remains at rest or moves at constant speed. If the constant speed is zero, this frame is called the rest frame of the particle.

The importance of the concept of an inertial system follows from the following idea (also called gedankenexperiment). A particle can be observed. If now the observer moves with respect to the particle, it will appear to be moving, even if it is the observer, which moves. Thus, the kinematics depend on the relative motion of observer and particle. However, if there are forces, i. e. something changing the kinematics, then there is a source of change not identical to just a change of coordinates, and therefore, no matter how, there is no coordinate system in which the particle behaves as expected.

There is one loophole to be fixed. If the observer would be accelerated, it may look like the kinematics change. Therefore, inertial systems are restricted to such systems which

may at most move relatively with a constant speed with respect to the coordinate system of the particle. If this is not the case, so-called pseudo forces, like the Coriolis force, emerge. This case will be discussed in section 2.11.1.

The abbreviated, sloppy, version of this law is: If there are no forces, the particle moves at constant speed (which includes zero speed).

2.2.3 The second law

Newton's first law identifies what happens in the absence of forces. Newton's second law describes what happens in the presence of forces. However, this requires first to define forces a little bit more. Note that this is indeed a definition of forces, not an explanation. This is one of the essences of theoretical physics, at least currently: It cannot explain everything in the sense of requiring nothing external. It can at best explain a multitude of experimental observations with a very limited number of external inputs. In this sense, also forces are something motivated and defined by experiment, but without derivation.

The definition is that a force is a vector, which is possibly time-dependent, $\vec{F}(t)$. This also implies that forces add like vectors, and the total force is the sum of all the individual forces. This is sometimes also called the fourth law, since this is also not something derivable.

In addition, every particle is assigned an inertial mass m , which is a property of said particle. There is no explanation of the origin of this mass in mechanics, and for any given problem the value of this mass has to be determined by experiment. This mass is an additive property, that is the mass of two particle M is just the sum of the individual particles' masses

$$M = m_1 + m_2,$$

and so on for more particles. This mass can have any arbitrary, positive value, and it is not quantized (comes in portions). It is an intrinsic property of a particle. In classical mechanics, furthermore, this property is immutable in time, $m(t) = m$.

Having these two concepts, the next step is, for the sake of convenience, to define a new quantity, the momentum of a particle,

$$\vec{p} = m\vec{v} = m\frac{d\vec{r}(t)}{dt}.$$

This will make the analysis especially of mass distributions, i. e. large numbers of particle with small masses, simpler, as well as the generalization beyond classical mechanics.

With this, it is possible to formulate the second law as

$$\vec{F} = \frac{d\vec{p}}{dt} = m\vec{a}(t) \tag{2.1}$$

i. e. the force changes the momentum and equals the acceleration up to a factor of the mass. As said, this is a definition, so there is no reason for it, except that it fits well with experiment.

Though mass is an immutable concept of a particle, it may still be useful to think of a time-dependent mass, e. g. if thinking of an ensemble of particles. When pouring particles on a scale, e. g., the mass on the scale changes. If this is the case, the second law takes the form

$$\vec{F} = \frac{d\vec{p}}{dt} = m(t)\vec{a}(t) + \vec{v}(t)\frac{dm(t)}{dt}, \quad (2.2)$$

i. e. the definition in terms of the momentum is the basic one, not the one in terms of the acceleration or the speed. This also elevates the momentum to be the central kinematical quantity in classical mechanics, and actually far beyond. This equation is also called the (Newtonian) equation of motion.

The equation is often also referred to as Newton's law or as the dynamical equation. While the first law and the third law describe only general features of systems with forces, it is this equation which actually describes the impact of forces on particles.

Though not explicitly noted, the force is in general not a constant, but it may (and in general will) depend on the position of the particles, as well as derivatives of the position, like the speed, the acceleration, or, in principle, even higher derivatives. In practice, the majority of cases involve only forces which are position-dependent, and sometimes dependent on the speed. Forces involving the speed are also often called frictional forces, as they usually appear in the context of friction phenomena.

The force may, in addition, depend also explicitly on the time, not only implicitly through the position of the particle as a function of time. This happens especially often if there is an external source of the force.

Because the force can then be seen as a function of other vectors, and has usually a well-defined value for every point in space and time, the force is often also considered a force-field, though the name force is still used for brevity. Only if the force does not depend on the position, but at most explicitly on time, is it strictly speaking not a force field.

2.2.4 The third law

The third law is of a substantially different nature than the two first laws. The two first laws describe how particles are affected by the presence or absence of forces, but do not make any statement of the origin of the forces. This is added by the third law. Its statement is that if the force on a particle emanates from another particle, then the target

particle acts always with the same but opposite force on the source particle,

$$\vec{F}_s = -\vec{F}_t,$$

i. e. any action induces a, equal in magnitude but opposite in sign, reaction. If there are more than two particles involved, this statement applies pairwise to each possible pairing of particles. Note that still no statement is made about how any of the involved particles creates the forces, but it requires for any possibility that this balance of action and reaction is satisfied. Again, there is no reason for this at the present time, since it is an axiom.

An important approximation is very often that it is assumed that a force is external. I. e., though the back reaction occurs, it is so weak that, for all practical purposes, the origin of the force is not changed, and therefore the force on the particle does not change. An example for this, discussed in detail in section 2.8.2, will be the movement of the earth around the sun. There, the impact of the third law can be taken exactly into account, but it can also be shown how it becomes irrelevant for the sun being much heavier than the earth.

2.3 Gravity

As noted before, Newton's laws do not explain the origin of the forces, just how they act on particles. They are therefore sometimes called a dynamical principle, but require still the force \vec{F} to actually describe motion. It is the realm of fundamental physics to deduce these forces from experiment, and investigate, which of these forces can be deduced from other forces. The most basic ingredients known today are general relativity and the standard model of elementary particles. Though not completely covering all experimental observations, all known forces can, in principle, be deduced from them. However, the actual derivation of, say, the forces involved in standing on a floor from these elementary theories is practically far too involved and too complicated. Therefore, rather than using them, it is much better to use effective forces, which neglect all those aspects which play no role, i. e. are too weak to make any practically measurable difference, rather than the full forces of these theories. This is then considered as an effective theory, rather than a, more or less, fundamental one. Especially, in the realm of classical mechanics only such effective forces play a practical role.

The probably best known of these effective forces is the gravitational force. Given the distance between two bodies, $|\vec{r}_1 - \vec{r}_2|$, the gravitational force between them is

$$\vec{F} = \frac{Gm_1^g m_2^g (\vec{r}_1 - \vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|^3}, \quad (2.3)$$

where $G \approx 6.6741(4) \text{ m}^3/(\text{kgs})$ is Newton's constant, a number obtained from measurement. The quantities m_i^g are the so-called heavy or gravitational mass. Just like the inertial mass, they are a property of a particles, and must be deduced by measurement. They act as a so-called charge, i. e. they are features of particles which determine the influence of a force on this particle. It is found experimentally that the gravitational masses are always positive.

It is a remarkable, and highly non-trivial, experimental finding that for a particle of inertial mass m and gravitational mass m^g

$$m = m^g$$

holds, i. e. gravitational and inertial mass are the same. This feature, also known as the equivalence principle, is the basis for general relativity, and thus one of the most basic foundations of modern physics. There is no explanation of it, though, it is again an axiom. However, since experimentally extremely well supported, in the following no more distinction between the gravitational and the inertial mass will be made.

There is an interesting special version of the gravitational force (2.3). Set one of the particles fixed at the coordinate origin, $\vec{r}_2 = \vec{0}$. Then

$$\vec{F} = m_1 G m_2 \frac{\vec{e}_r}{r^2} = m_1 \vec{g}$$

where the so defined vector \vec{g} is called the gravitational acceleration due to the body 2. E. g., on the surface of the earth, \vec{g} always points to the center of the earth and has a value, depending on latitude¹, of about 9.8 m/s. Since the radius of the earth is large, \vec{g} changes only very slowly when moving just a little bit vertically, and therefore can be taken to be roughly constant for the couple of kilometers, from the deepest ocean trench to the traveling altitudes of planes, where human activities usually take place.

2.4 Point particle

The simplest possibility is a constant force, \vec{F} . The equation of motion (2.2) then becomes for a constant-mass particle²

$$\frac{1}{m} \vec{F} = d_t^2 \vec{r}(t).$$

This is an ordinary differential equation of second order. It can be solved by integrating twice on both sides,

$$\vec{r}(t) = \int dt' \int dt'' \frac{1}{m} \vec{F} = \int dt' \left(\frac{t'}{m} \vec{F} + \vec{v}_0 \right) = \frac{t^2}{2m} \vec{F} + \vec{v}_0 t + \vec{r}_0, \quad (2.4)$$

¹Because the earth is not exactly spherical.

²For brevity, differential operators d/da will be abbreviated from now on by d_a , and $\partial/\partial a$ by ∂_a .

where the integration constants \vec{v}_0 and \vec{r}_0 describe the position and speed of the particle at time $t = 0$, and are the so-called initial conditions of the motion. Since the equation of motion is an ordinary second-order differential equation there are always two such initial conditions required to fully specify the solution of the equation.

If the force vanishes, $\vec{F} = \vec{0}$, the particle moves at constant velocity. In this sense, Newton's first law is actually just a special case of Newton's second law, though the definition of an inertial system will play a quite central role later.

An interesting observation is the following. Because the equation is linear, adding two forces \vec{F}_i will yield that the movement of the particle will be just the sum of the effects of the two forces,

$$\vec{r}(t) = \frac{t^2}{2m}(\vec{F}_1 + \vec{F}_2) + \vec{v}_0 t + \vec{r}_0.$$

This is called a superposition of the two movements, where the consequences of the initial conditions can be taken to be also the sum of two initial conditions, for each movement separately.

The reason is of mathematical nature. If a differential equation is linear and homogeneous, i. e. is of the type

$$\sum_{i=1}^N a_i d_t^i \vec{r} = \vec{0},$$

then any linear combination of two solutions (of which there are N for an ordinary differential equation of order N) again solves this equation. If there is any inhomogeneity on the right-hand side, then an arbitrary solution for this equation is given by any solution of the inhomogeneous equation to which any linear combination of the homogeneous solutions can be added.

Note that this is a particularity of linear differential equations. If, e. g., \vec{r}^2 would appear, this is no longer true. However, situations where (2.2) is a linear differential equation, with or without inhomogeneous term, are very common in classical mechanics, and therefore this superposition principle will play an important role.

An interesting example is the situation with friction. Then $\vec{F} = \alpha d_t \vec{r}$, where α is a friction coefficient. The equation of motion (2.2) is then

$$d_t^2 \vec{r} - \frac{\alpha}{m} d_t \vec{r} = 0.$$

This requires that the derivative of the first derivative must again be proportional to the first derivative. This is the typical behavior of the exponential function, and the solution is thus

$$\vec{r}(t) = \frac{m}{\alpha} \vec{v}_0 e^{-\frac{\alpha t}{m}} + \vec{r}_1,$$

where the two initial conditions give again the speed and position of the particle at $t = 0$. The two solutions are now both terms. Either being at rest from the beginning, or its movement being exponentially damped.

2.5 The potential

An interesting concept can be found when considering the movement of a particle under an arbitrary, but only position-dependent, force. It is best to start with a one-dimensional example first. The equation of motion then reads

$$md_t^2x = F(x).$$

Multiplying this equation by d_tx , this yields

$$m(d_tx)(d_t^2x) = F(x)d_tx. \quad (2.5)$$

It can now be recognized that both sides can be rewritten as derivatives

$$d_t \left(\frac{m}{2} (d_tx)^2 \right) = d_t \int F(x') dx' = -d_t V(x), \quad (2.6)$$

where the quantity $V(x)$, being the primitive of $F(x)$, has been introduced. Note that any integration constant in $V(x)$ does not play a role, as the time derivative removes it immediately. This primitive is called the potential, which generates the force. The appearing minus sign is a matter of convention.

It will happen very often that not the force, but the potential is known. The force can then be obtained by

$$F(x) = -d_x V(x), \quad (2.7)$$

i. e. the derivative of the potential is the force. This again shows that any constant terms in $V(x)$ do not play a role, and can be chosen at will. Such a kind of arbitrariness seems to be at first quite astonishing, since nature should be somehow uniquely determined. There is, however, a deeper reason behind this arbitrariness, which will become evident during the lecture. However, it is best to postpone a deeper discussion of it until more conceptual progress has been made.

Since on both sides of (2.6) total derivatives appear, the equation can be integrated to yield

$$\frac{m}{2} (d_tx)^2 = E - V(x), \quad (2.8)$$

where E is an integration constant. Note that this integration constant, which emerges from a time and not a spatial integration, cannot be dismissed. Its relevance will be

discussed in more detail below. Before doing this, it is possible to solve this equation by separation of variables, yielding an implicit result

$$t - t_0 = \int_{x(0)}^{x(t)} \frac{dx'}{\sqrt{\frac{2}{m}(E - V(x'))}}, \quad (2.9)$$

which after evaluation of the integral can then be solved for $x(t)$ to get the final solution. This solution is parametrized by the constant E and the initial condition $x(0)$. Thus, these are taking the role of the two initial conditions of position and speed at time zero used before.

Before continuing, as a brief remark the situation in more than one dimension is a little more involved. In general, any potential $V(\vec{x})$ will create a force field

$$\left(\vec{F}(\vec{x})\right)_i = -\partial_{x_i} V(\vec{x}),$$

as can be seen by performing the steps above for every component. In the example of the point particle in section 2.4, the potential for the constant force is $\vec{F}\vec{x}$.

However, this means that a single function must create as many different functions as there are dimensions. In general, this is not possible. A criterion when this is possible will be developed later. In general, if it is possible, the force is said to be conservative. Also, if the force depends explicitly on time or on speed, it is in general not possible to find a potential, and the force becomes even in one dimension non-conservative. It is an amazing, and not understood, feature of nature that eventually on the most basic level all experimentally established forces are conservative. However, this feature may be hidden if only an effective description not in terms of the elementary forces is performed. This is called an apparent non-conservative forces, and many examples are known in daily life.

While so far only the indefinite integral has been used, it is also possible to use the definite integral

$$W_{12} = \int_{x_1}^{x_2} dx F(x) = V(x_1) - V(x_2).$$

This quantity is the necessary integrated force to move something between the two points x_1 and x_2 . It is therefore called the work which has been done. It corresponds to the difference in potential. The potential therefore describes the amount of work which can be done, and actually doing some work is reducing the potential. Conversely, investing work raises the potential. Thus, the name potential. The amount of stored work for a particle at a position x with respect to zero potential is called the potential energy. In the general

case, this will be a line integral, i. e.

$$W_{12} = \int_{\vec{x}_1}^{\vec{x}_2} d\vec{x} \vec{F}(x) = V(\vec{x}_1) - V(\vec{x}_2), \quad (2.10)$$

but will remain a scalar quantity.

If in equation (2.8) the potential is set to zero, the constant E is entirely giving by a quantity obtained from the motion of the particle. On the other hand, solving for E of (2.8) yields

$$E = \frac{m}{2}(d_t x)^2 + V(x). \quad (2.11)$$

For a particle at rest, E is then the potential energy. Thus, in general, E is called the total energy, combining the potential energy $V(x)$ and a contribution from the motion of the particle $m(d_t x)^2/2 = p^2/(2m)$ which is called the kinetic energy, and where p is again the momentum. In more than one dimension this kinetic energy, often abbreviated as T , is given by

$$T = \frac{m}{2}(d_t \vec{r})^2 = \frac{\vec{p}^2}{2m}.$$

Once more, the definition using the momentum is the more general one, as it can also cope with the situation of a time-dependent mass.

Because of the general solution (2.9), the sum $E - V$ of a particle must be positive at every point in space, since otherwise there is no solution. Thus, a particle needs to have a positive or zero kinetic energy. Furthermore, when $E = V(x)$ for some point x , the kinetic energy has to vanish, as it is a positive quantity. The second derivative may not vanish, and therefore the particle does not necessarily stops there. If the potential further increases to one side, it will actually be deflected there, a so-called inflection point of the movement. Note that the prediction of this behavior did not need the solution of the equation of motion. In fact, the energy will become a very convenient tool to simplify calculations later.

Another interesting situation arises if the potential has a minimum or a maximum at some point x . At these points, the force, being the derivative of the potential, necessarily vanishes. Thus, a particle set at such a position at rest will remain so indefinitely, since no force acts. If the extremum is a minimum, the force to either side of the minimum always point in the direction of the minimum. Thus, if the particle at rest is only slightly disturbed, it will return to the minimum, and move around it if there is no dissipation. This is called a stable equilibrium. At a maximum, however, the force points away from the maximum. Any slight disturbance of the particle at rest will therefore accelerate it

away from the maximum. This is thus an unstable equilibrium³.

One of the probably most fundamental statements in mechanics is that the energy is x -independent, which follows from (2.8), but also time-independent for conservative, i. e. t -independent, potentials. This follows from (2.5)

$$d_t E = d_t \left(\frac{m}{2} (d_t x)^2 + V(x) \right) = m(d_t x)(d_t^2 x) - F(x)d_t x = 0. \quad (2.12)$$

If the potential depends on time or speed, i. e., it can be written as

$$F(x) = d_x V(x) + f(x, d_t x, t),$$

the energy changes with a rate of $f(x, d_t x, t)d_t x$.

Again, in one dimension any force, which is time and speed independent, has a potential. This is not so simple in more than one dimension. To test, when this is possible, note that (2.10) implies that if a potential exists $W_{11} = 0$, no matter the path, or

$$\int_{\mathcal{C}} d\vec{x} \vec{F}(x) = 0,$$

for any closed curve \mathcal{C} . There is a powerful theorem in functional analysis, which guarantees that this is equivalent to the requirement⁴

$$\epsilon_{ijk} \partial_{x_j} F_k = 0$$

for all i , which is much simpler to check than the integral condition. However, this equivalence is only true, if the force is continuously differentiable, or at least if the curve can be contracted to a point without crossing any singularities. This condition also implies

$$\partial_{x_i} \partial_{x_j} V(\vec{x}) = \partial_{x_j} \partial_{x_i} V(\vec{x}),$$

for any combination of i and j , and thus requires that the potential is (at least) twice continuously differentiable. Note that a potential can always be used to find a force, but this force may not everywhere be well-defined, if the potential is not always continuously differentiable.

³If the force is very weak around the maximum, e. g. if it is maximum of higher order, the acceleration away will be very slow. Such situations are sometimes called metastable, though there is no firm definition of when an unstable situation becomes metastable.

⁴Note that here and hereafter the Einstein convention is used that over any pairs of indices in a given term a sum is performed over their full range, if not stated otherwise.

2.6 Harmonic oscillator

Probably the most important problem in mechanics is the harmonic oscillator. In its simplest form in one dimension, this is the situation if the force is negatively proportional to the distance of the particle from the origin, i. e.

$$d_t^2 \vec{r}(t) = -\frac{\alpha}{m} \vec{r}.$$

E. g., a spring, obeying Hooke's law, will create such a force. The associated potential is $\alpha \vec{r}^2/2$.

The solution of this equation requires two functions which, up to a negative constant, will turn into itself when differentiating twice, to yield the two solutions. Such functions are given by sine and cosine. Therefore, a solution is

$$\begin{aligned} \vec{r}(t) &= \vec{r}_0 \cos(\omega t) + \frac{\vec{v}_0}{\omega} \sin(\omega t) \\ \omega &= \sqrt{\frac{\alpha}{m}}, \end{aligned} \quad (2.13)$$

where the two initial conditions \vec{r}_0 and \vec{v}_0 are used to fix the position and speed at time $t = 0$, respectively.

There is an alternative way to solve this equation, which looks at first somewhat unusual, but is in fact a very important technical trick. A possible solution is also given by

$$\vec{r}(t) = \Re \left(\left(\frac{\vec{r}_0}{2} + \frac{\vec{v}_0}{2i\omega} \right) e^{i\omega t} + \left(\frac{\vec{r}_0}{2} - \frac{\vec{v}_0}{2i\omega} \right) e^{-i\omega t} \right).$$

By expanding the exponentials using Gauss' formula, it becomes evident that this is exactly the same as (2.13). There is no advantage in this particular case, but as will be seen, in more general cases this will be very useful.

Another interesting feature is obtained when considering the more general case of a driven accelerator with friction, described by the equation of motion

$$d_t^2 \vec{r}(t) + \frac{\beta}{m} d_t \vec{r}(t) + \frac{\alpha}{m} \vec{r} = \vec{a} \sin(\sigma t + \phi). \quad (2.14)$$

To solve this equation, it is best to start with the homogeneous case first, i. e. with $\vec{a} = 0$. It is in this case where the usage of the exponentials becomes interesting. Make the ansatz $\exp(at)$, and insert it into the equation of motion. This yields a quadratic equation for a with the solutions

$$a_{\pm} = \frac{1}{2m} \left(-\beta \pm \sqrt{\beta^2 - 4\alpha m} \right).$$

The solution for the homogeneous case will then be

$$\vec{r}_0(t) = \Re \left(\left(\frac{a_- \vec{r}_0 - \vec{v}_0}{a_- - a_+} \right) e^{a_+ t} + \left(\frac{a_+ \vec{r}_0 - \vec{v}_0}{a_+ - a_-} \right) e^{a_- t} \right).$$

The resulting path then depends on the relative sizes of the involved constants. There are three distinct cases, depending on the value of a_{\pm} .

If $\beta^2 < 4\alpha m$, the argument of the squareroot becomes negative, and the a_{\pm} are complex. If β is positive, this corresponds to a superposition of an exponential damping, and an oscillation. Thus, after an initial stage, the motion becomes that of an ordinary harmonic oscillator, though with a frequency depending on the interplay of damping and the force and a exponentially decreasing amplitude. If β is negative, however, the movement becomes exponentially increasing. This happens, if the friction term enhances motion. Thus, such a term destabilizes the motion.

If the argument exactly vanishes, the movement will be exponentially damped, and degenerate. In this case, the time-dependence can be factored out, and the denominator vanishes.

If the argument is positive, the solution a_+ will again yield an exponentially increasing motion, while a_- an exponentially decreasing one. It depends on the initial conditions, which one will eventually win. However, there is no oscillatory behavior.

Note that the friction force can exponentially increase the motion. But this is no longer really friction, as it provides energy to the system.

If the equation of motion (2.14) \vec{a} no longer vanishes, the result is

$$\begin{aligned} \vec{r}(t) &= \vec{r}_0(t) - \vec{d}(t) + \vec{d}(0) \\ \vec{d}(t) &= \vec{a} \frac{m}{(m\sigma^2 - \alpha)^2 + \beta^2\sigma^2} (\beta\sigma \cos(t\sigma + \phi) + (m\sigma^2 - \alpha) \sin(t\sigma + \phi)), \end{aligned}$$

which exhibits again the structure of being the solution to the homogeneous equation plus an explicit solution of the inhomogeneous equation. The important addition is the driving term \vec{d} , since for \vec{r}_0 just the previously stated behavior emerges again. This can be seen to be the necessary inhomogeneous part for the solution by entering it into the solution. It is a reasonable ansatz, as it has the same form as the driving term, but in the end, this is here an educated guess.

If $\beta = 0$, this term diverges if $m\sigma^2 = \alpha$. Thus, close to this value, the amplitude grows beyond any bounds, and therefore totally dominates the result. This is called a resonant behavior, or just a resonances. Physically, what happens is that the external force applies just exactly such that it always accelerates the movement a little bit further, instead of damping it occasionally. Thus, the motion grows beyond any bound.

If $\beta \neq 0$, there is no divergence, but still a strong enhancement at $m\sigma^2 = \alpha$. This is called a damped resonance. Considering the prefactor as a function of α , the width is defined as the amount of deviation of α from the critical value $\alpha = m\sigma^2$ where the function drops to a half⁵. This width is $2(\beta^2\sigma^2 + 2m^2\sigma^4)^{1/2}$.

Similar (damped) resonances are a feature exhibited by many physical system. Understanding it well for the harmonic oscillator is therefore understanding a prototype for a multitude of physical phenomena, from celestial mechanics to particle physics.

Note that ϕ only acts as phase, i. e. it modifies only to some extent the relative behavior of the two oscillations, if also \vec{r}_0 shows an oscillatory behavior.

More interesting is that the maximal amplitude is reached no longer when \vec{r}_0 reaches it maximum, but delayed by a so-called phase shift γ . The value of this phase shift depends on the value of α when all other quantities are fixed. It is trivially zero for $\alpha = 0$, as then all oscillation is just given by the driving force. It can be shown to be negative for all values of α , becoming $-\pi/2$ at the resonant frequency, and tends to $-\pi$ for α to infinity. If β is zero, it actually jumps from zero to $-\pi$ at the resonant frequency, and this jump becomes smoothed out the larger β becomes.

2.7 Central potential

Generically, forces on particles of the type

$$\vec{F} = f(\vec{r}, d_t\vec{r}, \dots, t)\vec{r}, \quad (2.15)$$

i. e. having the same direction as the vector \vec{r} , are called central forces. These forces assume that the source of the force is at the center of the coordinate system, and that the direction of the force is towards this center. The further crucial assumption is that there are no lateral forces, so that the prefactor only involves the distance. These forces are probably the most important type, especially in astrophysics, since gravity, (2.3), is the probably best known example. Their structure also entail many further consequences, which are prototypical. They shall therefore be treated in some detail.

As a first step, it is useful to find the condition under which there is a potential for these forces. The first condition is that the function f is at most depending on \vec{r} , to avoid any dissipation. Furthermore

$$0 = \epsilon_{ijk} d_{r_j} F_k = \epsilon_{ijk} ((d_{r_j} f) r_k + f \delta_{jk}) = \epsilon_{ijk} r_k (d_{r_j} f)$$

⁵Sometimes also the value is determined when it drops to $1/e$ or to $\ln 2$, depending on the context. These are then different numbers than for the factor 2.

This condition can only be fulfilled, if the derivative is proportional to r_j , which will only happen if f depends only on $|\vec{r}|$,

$$d_{r_j} f(|\vec{r}|) = d_x f(x) d_{r_j} |\vec{r}| = d_x f(x) \frac{r_j}{|\vec{r}|}.$$

Thus, a conservative central force must be of the form $f(r)\vec{r}$, where $r = |\vec{r}|$ for brevity.

2.7.1 Angular momentum

For the following, it is useful to first introduce a further concept, angular momentum. Take the equation of motion (2.2), and form a vector product with \vec{r} , yielding

$$(\vec{M})_i = \epsilon_{ijk} r_j F_k = m \epsilon_{ijk} r_j d_t^2 r_k = d_t(m \epsilon_{ijk} r_j d_t r_k) = d_t(\epsilon_{ijk} r_j p_k) = d_t l_i. \quad (2.16)$$

The so defined quantity \vec{l} is called the angular momentum, whose time evolution is determined by the torque \vec{M} . This is called the angular momentum law. If there is no torque, because either the force itself vanishes or has a vanishing vector product with the position, the angular momentum is conserved, as its time derivative vanishes.

However, the actual value of the angular momentum is not intrinsic to the system, but depends on the coordinate system. This can be seen from the free particle. Since the force vanishes, so does the torque. But the position vector and the speed need not be parallel, but can be, depending on the coordinate system, though it is always constant. Thus, a statement about the value of the angular momentum requires to also provide the coordinate system. The rate of change, however, is physical, as it is uniquely given by the torque.

For a central force, (2.15), the torque always vanishes, and the angular momentum is conserved. This is the reason why it will be so relevant in this section.

A useful first consequence is the geometrical interpretation of the angular momentum, which can be derived from its magnitude

$$\frac{1}{2m} |\vec{l}| = |\epsilon_{ijk} r_i d_t r_j e_k|. \quad (2.17)$$

The right hand side has dimension area per time. Geometrically, it is the area which the vector pointing from the origin to the particle covers per unit time. If angular momentum is conserved, this area is constant. As will be seen, e. g. the planets fulfill this so-called area theorem.

2.7.2 Effective potential

For a conservative central potential both the energy (2.11) and the angular momentum (2.16), and especially its length $l = |\vec{l}|$, are conserved. This can be used to simplify the solution of the equations of motion.

First, because the angular momentum is conserved the speed and the position are coplanar in a temporally constant plane, since

$$\vec{r}\vec{l} = d_t\vec{r}\vec{l} = \vec{0},$$

since the cross product is perpendicular to its components. Thus, it is possible to restrict the description to a plane. Due to the radial symmetry it is convenient to choose angular coordinates for the description, i. e. a distance from the origin r (on which the potential depends) and an angle ϕ , thus $x = r \cos \phi$ and $y = r \sin \phi$.

This implies

$$\begin{aligned} E &= \frac{m}{2}(d_t\vec{r})^2 + V(r) = \frac{m}{2}((d_tr)^2 + r^2(d_t\phi)^2) + V(r) \\ &= \frac{m}{2}(d_tr)^2 + \frac{l^2}{2mr^2} + V(r) = \frac{m}{2}(d_tr)^2 + V_e(r). \end{aligned} \quad (2.18)$$

This result has a number of interesting implications. First, the energy is entirely determined by the radius r as a function of time, i. e. the distance from the origin. Its angular position is not relevant. Secondly, the situation is analogous for the one-dimensional particle of section 2.5, but with the modified, the so-called effective, potential V_e , rather than the original potential V .

The angular motion can be determined from

$$d_t\phi(t) = \frac{lr^2}{m}, \quad (2.19)$$

as a consequence of the conservation of the angular momentum. Thus, the full solution are now obtained from two differential equations of the first kind, rather than of the second kind. In analogy to section 2.5, both equations can be integrated to yield

$$t - t_0 = \int_{r(0)}^{r(t)} \frac{dr'}{\sqrt{\frac{2}{m}(E - V_e(r))}} \quad (2.20)$$

$$\phi - \phi_0 = \int_{r(0)}^{r(\phi)} \frac{ldr'}{r'^2 \sqrt{2m(E - V_e(r'))}}, \quad (2.21)$$

yielding the (implicit) solution, as a function of two more integration constants, r_0 and ϕ_0 . They come about as Newton's law is originally a second order differential equation,

and for two variables thus needs four integration constants, being here E , l , r_0 and ϕ_0 . Of course, if wished, a uniform motion in the z -direction can be superimposed with this solution.

2.7.3 Planetary motion

This previous result is fully general. It is, however, quite interesting to study the case of $V(r) \sim 1/r$ in more detail. This particular case is of special importance as there are two situations in which it arises.

One is the electrostatic force, where it takes the form

$$V(r) = -\epsilon \frac{q_1 q_2}{r},$$

where ϵ is a constant depending on the system of units chosen, and this is the potential between two electric charges having electric charges q_1 and q_2 respectively.

The other one is Newton's law of gravity,

$$V(r) = -\gamma \frac{mM}{r},$$

and describes the potential between two bodies of masses m and M , and γ is again a system-of-units-dependent constant, called Newton's constant.

In both cases it is tacitly assumed that one of the bodies resides at the center of the coordinate system. Otherwise, r has to be replaced by $|\vec{r}_1 - \vec{r}_2|$, the distance between both bodies. In the following it will be furthermore assumed that the body at the origin will not move. This is an excellent approximation if one of the bodies is much heavier than the others. This is e. g. true if the two bodies are the sun and the earth, a satellite and the earth, or an atomic nucleus and an electron. If this is not true, this becomes a two-body problem which, in this particular case, can actually be solved only with slightly more effort. This will be done in section 2.8.2. However, since this only obscures a few things right now, this will be postponed until later, and the approximation will be made.

It should be noted that, though this is called Newton's law of gravity, there is a-priori no casual connection between this law and Newton's three laws (except that they have been discovered by the same person, Newton). The first three laws are about inertial masses. This law is about the gravitational masses. It is, as noted above, only an experimental result that these two masses are identical.

Though this problem can be solved with the methods of the previous section 2.7.2, it is useful to take the opportunity to demonstrate also a different, but equally useful, way of solving the problem: Another replacement of variables.

To start out, define $s = 1/r$. Though s is a function of the time t , it is also possible to consider it rather as a function of the angle ϕ in the same two-dimensional coordinate systems as in section 2.7.2. Then the chain rule yields

$$\frac{ds}{d\phi} = \frac{d\frac{1}{r}}{dt} \frac{dt}{d\phi} = -\frac{d_t r}{r^2} \frac{mr^2}{l}$$

where (2.19) has been used. Inserting this into (2.18) yields

$$E = \frac{l}{2m} ((d_\phi s)^2 + s^2) + V(s).$$

Though it may appear tempting to directly solve this equation, it is in this case better to take a detour, born from hindsight and experience.

Differentiating this equation a second time with respect to ϕ yields

$$0 = \frac{l^2}{2m} (2(d_\phi s)(d_\phi^2 s) + 2sd_\phi s) + (d_s V(s))(d_\phi s) = d_\phi s \left(\frac{l^2}{2m} (2(d_\phi^2 s) + 2s) + d_s V(s) \right).$$

This equation has one solution with $ds/d\phi = 0$, i. e. r is constant as a function of ϕ . This is a perfect circular orbit. The term in parentheses is also a linear differential equation of second kind

$$\frac{l^2}{2m} (2(d_\phi^2 s) + 2s) + d_s V(s).$$

Furthermore, the derivative of V with respect to s is just a constant, and therefore the equation is

$$d_\phi^2 s + s = \frac{\gamma m^2 M}{l^2}. \quad (2.22)$$

This shows the motivation for this approach. Out of a non-linear differential equation the task has been reduced to the task of solving two linear differential equations, which is far simpler in general.

But equation (2.22) is already known. It is one particular version of the harmonic oscillator equation of section 2.6. Thus, the solution can be read off directly by replacing t in section 2.6 by ϕ , and yields

$$s(\phi) = \alpha \sin \phi + \beta \cos \phi + \frac{\gamma m^2 M}{l^2},$$

where the constants α and β have to be fixed by initial conditions. A convenient choice is to select $\alpha = 0$, which implies that the minimal value of r is at $\phi = 0$, if $\beta > 0$. The solution is then given by

$$\begin{aligned} s &= \frac{1}{r} = \beta \cos \phi + \frac{\gamma m^2 M}{l^2} = \frac{1}{k}(1 + \epsilon \cos \phi) \\ k &= \frac{l^2}{\gamma M m^2} \\ \epsilon &= \beta k \end{aligned}$$

where the last rewriting is convenient to characterize the geometric properties of the solution. These are just cone cuts, and for ϵ smaller, equal, or greater than 1 this describes an ellipsoid, a paraboloid, and a hyperboloid. Note that the case $\beta = 0$ returns exactly the circle case. Thus, ϵ is also called the eccentricity of the orbit. Thus, the quality of the solution is entirely characterized by ϵ .

The case of $\epsilon < 1$ (with $\epsilon = 0$ being the circle) is just the ordinary case of a planetary orbit around the sun. This can be seen from the fact that $(1 + \epsilon \cos \phi)$ remains bounded, and hence so does r . At the same time, the motion is periodic.

If $\epsilon = 1$, then the motion is no longer periodic, since now s can vanish for $\phi = \pi$. Still, ϕ can still reach all values, especially zero, and therefore the movement is a parabola. It is an ellipsoid of which one of the main axes goes to infinity.

If $\epsilon > 1$, then there is no longer a positive solution for r for all values of ϕ . It can therefore no longer be an ellipsoid. This implies that not all ϕ values are allowed, and the path of the particle becomes a hyperbola: The particle tries to approach the central one, but is deflected before it can reach it. The point of closest approach is given by $r = k/(1 + \epsilon)$.

It is quite instructive to return to the energy of the particle. Since the kinetic energy is always positive, it follows from (2.18)

$$E \geq \frac{l^2}{2mr^2} - \frac{\gamma mM}{r}.$$

If the energy is greater than zero, this equation has a solution for all r greater than some limiting r_0 , which vanishes for $l = 0$. This implies that a particle with positive energy corresponds to the hyperbola. A non-vanishing angular momentum increases the point of closest approach r_0 . Therefore it is said that the angular momentum creates an angular momentum barrier. If E is exactly zero this is the smallest possible value for which it is still possible to have an infinite distance. It is therefore corresponding to the parabola. If the energy becomes negative, the equation has no solution also for r larger than some value r_1 , the movement is therefore bounded. This corresponds again to the closed orbits. Since in general $r_0 \neq r_1$, the orbit is an ellipsoid. For the smallest possible value of the energy, $r_0 = r_1$, and the motion becomes the circular orbit.

Thus, even without solving the system, it would have been possible to determine many qualitative features of the particle's motion just by studying (2.18). Such studies therefore are an extremely important tool. If, e. g., the potential would have taken the value $V(r) = r$, a similar study would immediately yield that the particle can never move to $r = \infty$.

In the whole discussion, the time-dependence was not an issue. If the time-dependence

is actually of relevance, it can be obtained from (2.19). However, the actual solution is rather involved.

Still, from the results the famous laws of Kepler can be deduced for planetary, i. e. bounded, motion. Since the heavier mass is at the origin the planets move along ellipsoids with the sun at one of the focus points. The relation (2.17) is actually already Kepler's second law if angular momentum is conserved, as it is here.

Kepler's third law states that the ratio between the time needed for a complete orbit T squared and the third power of the larger axis is constant. It appears that this would require to have the time dependence, but this is not the case. The area of the ellipse is, using (2.17),

$$\pi ab = \frac{Tl}{2m}$$

But the value of b is just given by the minimal value of s at $\pi/2$. Thus follows

$$\frac{T^2}{a^3} = \frac{4\pi^2}{\gamma M},$$

which completes the proof.

2.8 Mass distributions and center of mass

2.8.1 General properties

The previously discussed situation with two particles is a special case of having N particles. It is useful to discuss this situation in some detail, as it appears quite often, e. g. when looking at the total solar system.

Let each of the particles have its own mass m_i . Because of Newton's third law the force \vec{F}_{ij} with which particle i acts on particle j , e. g. by gravitation, must obey $\vec{F}_{ij} = -\vec{F}_{ji}$. Of course, a particle does not act on itself, and thus for simplicity $\vec{F}_{ii} = \vec{0}$. There can be also external forces on the individual particles \vec{F}_i . For the solar system, this may be the gravitational pull of the galaxy as a whole.

There are thus dN equations of motion, where d is the number of dimensions⁶,

$$m_i d_t^2 \vec{r}_i = \vec{F}_i + \sum_j \vec{F}_{ij}.$$

Consider now the sum of all N equations of motion,

$$\sum_i m_i d_t^2 \vec{r}_i = \sum_i \vec{F}_i, \quad (2.23)$$

⁶There may also exist genuine n -body forces, which involve non-separable function of more than two coordinates. This only complicates the remainder unnecessarily, but can appear in practice.

and thus the internal forces do not appear. Define furthermore

$$\begin{aligned} M &= \sum_i m_i \\ \vec{R} &= \frac{1}{M} \sum_i m_i \vec{r}_i \\ \vec{f} &= \sum_i \vec{F}_i. \end{aligned}$$

The equation (2.23) then reads

$$M d_t^2 \vec{R} = \vec{f},$$

which looks just like a single-particle equation of motion. Therefore, the center of mass \vec{R} moves like a single particle having the total mass M only under the influence of the external forces. It does not matter how involved the internal forces are for this, they do not appear.

It may also be useful to define analogously a total momentum and angular momentum,

$$\begin{aligned} \vec{P} &= \sum m_i d_t \vec{r}_i = \sum \vec{p}_i \\ \vec{l} &= \sum m_i \epsilon_{ijk} r_i d_t r_j \vec{e}_k = \epsilon_{ijk} R_i P_j \vec{e}_k + \sum_i \epsilon_{ijk} (r_i - R_i) (p_j - P_j) \vec{e}_k = \vec{L} + \sum \vec{l}_i \end{aligned}$$

where \vec{L} is the angular momentum of the center of mass while the \vec{l}_i are the relative angular momentum with respect to the center of mass. Furthermore, if all forces are conservative then in analogy to the single particle a potential energy can be defined, where it useful to define separately the potential between two particles and of the external forces separately. Especially, for a two-particle potential it holds that

$$\begin{aligned} \vec{F}_{jk} &= \vec{e}_i d_{\Delta \vec{r}_i} V_{jk}(\Delta \vec{r}) \\ \Delta \vec{r} &= \vec{r}_j - \vec{r}_k \end{aligned}$$

and thus the forces are obtained by deriving with respect to the connecting vector. This implies that the potentials are superimposed like the forces, i. e. the total potential of a mass particle is the sum of all potentials acting on it.

2.8.2 Two-particle systems

Of particular practical importance is the situation when $N = 2$, i. e. there are two particles only. The center-of-mass is then

$$\vec{R} = \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2}.$$

The vector $\vec{r} = \vec{r}_1 - \vec{r}_2$ gives the relative distance between both particles. It is now possible to rewrite the position of the particles in terms of relative coordinates and the center-of-mass coordinates only,

$$\vec{r}_1 = \vec{R} + \frac{m_2}{M} \vec{r} \quad (2.24)$$

$$\vec{r}_2 = \vec{R} - \frac{m_1}{M} \vec{r}. \quad (2.25)$$

The center-of-mass movement is as before determined by the external forces only. The equation of motion for the relative coordinate is

$$d_t^2 \vec{r} = \frac{\vec{F}_1}{m_1} - \frac{\vec{F}_2}{m_2} + \frac{\vec{F}_{12}}{m_1} - \frac{\vec{F}_{21}}{m_2}.$$

The dependence on the masses suggests to define the so-called reduced mass

$$\mu = \frac{m_1 m_2}{m_1 + m_2}.$$

In terms of this mass the equation of motion becomes

$$d_t^2 \vec{r} = \frac{\vec{F}_1}{m_1} - \frac{\vec{F}_2}{m_2} + \frac{\vec{F}_{12}}{\mu}.$$

If the external forces vanish, what is called a closed system, the equation of motion for the relative coordinate no longer references the external system. Furthermore, it can be shown that also the relative angular momentum takes the form $\vec{l} = \mu \vec{r} \times d_t \vec{r}$. Thus, the equation of motion for the relative coordinate is the same as for a single particle with the reduced mass.

If one particle is much heavier than the other the reduced mass is essentially identical to the mass of the lighter particle. Thus, in this formulation the approximation made in section 2.7.3 becomes more transparent. Since the planet (or satellite) is so much lighter than the sun (the planet), the reduced mass is essentially that of the planet (the satellite). Thus, the equation of motion for the relative coordinate is essentially the one in the case of the fixed heavier particle. However, with the formulation developed here, it is possible, using equations (2.24-2.25), to determine the actual movement of both bodies, but this requires to solve only the one-particle problem. By direct comparison, this is much simpler: It now only necessary to substitute in all results of section 2.7.3 the mass of the planet by the reduced mass, and the result is automatically the correct one for the two-body problem.

Of course, the substitution can be done for either of the bodies. Thus, both bodies will perform exactly the same type of movement. In particular, for a bounded planetary

motion both celestial bodies will have an orbit around the same point, which is the center of mass. Superimposed to the orbital motion of both bodies can then be a movement of the center of mass.

This is also the way how Newton's third law seems to have no impact on the source of the force, as announced in section 2.2.4: The reduced mass is so close to the earth's mass that setting it equal to the earth's mass does not create an appreciable error. On the other hand, the force on the sun is so tiny that its movement is all but negligible. Thus, while in the closed system Newton's third law holds, its violation by setting the external force constant and immutable is a very good approximation. This also justifies to make this approximation in more involved cases, where the backreaction is known to be small, but its details too involved to be included, a situation arising quite often in practice.

It is unfortunate insight that a similar reduction of complexity is not possible if there is more than two objects involved. The three(and more)-body problem cannot be reduced to a one-body problem, but a full solution is required. E. g. the movement in the solar system or of the solar system around the center of the galaxy is such a three, or more, body problem. However, in these cases it is possible to simplify the problem, see section 2.9.

2.8.3 Scattering

A situation which is of high relevance in many physical application is a closed system such that the two-body potential (or a force) is short-range. This can happen in either of two cases. One possibility is that the potential has a sharp cut-off, $V(\Delta\vec{r}) \propto \theta(|\Delta\vec{r} - \vec{r}_0|)$, where the value \vec{r}_0 belongs to the definition of the potential. The other is that it decays fast enough. What fast enough means is rather context-dependent, but very often requires at least an exponential decay at large distances, $\exp(-|\Delta\vec{r}|/r_0)$, where the scale r_0 is once more characteristic for the potential, but even maybe some kind of power-law dependence $1/|\Delta\vec{r}|$ is sometimes sufficient.

In such a situation it is possible to define a scattering process in the following way. Start out with two particles, which are initially so far separated that they are not interacting. They are then send towards each other in such a way as their center of mass is at rest⁷. They afterwards escape again to infinity, and stop interacting.

No matter how the details of this kind of interaction is, there are a number of conservation laws, which are necessarily fulfilled, if the interactions are conservative, which is

⁷This is not necessary but makes the following calculations much simpler.

called elastic scattering. Especially, the linear momentum has to be conserved,

$$\vec{p}_1 + \vec{p}_2 = \vec{p}'_1 + \vec{p}'_2,$$

where the primes denote the situation after the scattering. By construction, the initial relative momentum is zero, $\vec{p}_1 + \vec{p}_2 = \vec{0}$. Therefore, the final momentum must also be zero. Furthermore, this implies that the direction is arbitrary, and can therefore be selected at will.

Furthermore the energy is conserved. Since in the beginning there is no potential energy, it follows that

$$T = \frac{\vec{p}_1^2}{2m_1} + \frac{\vec{p}_2^2}{2m_2} = \frac{\vec{p}'_1{}^2}{2m_1} + \frac{\vec{p}'_2{}^2}{2m_2} = T'.$$

Since $\vec{p}_1 = -\vec{p}_2$, $\vec{p}_1^2 = \vec{p}_2^2 = \vec{p}'_1{}^2 = \vec{p}'_2{}^2$.

These conditions enforce that the incoming and outgoing momenta both lie along respective lines. Hence, all movement is contained in a plane, and the coordinate system can be chosen such that all components in the third direction can be chosen to be zero. Thus, there remain only two components for the final momenta free. One is constrained by the energy conservation, leaving only one component. This can be traded in for the relative angle between the incoming and outgoing momentum, θ . Thus, the only freedom left by the kinematics is the relative angle between one of the incoming and one of the outgoing momenta. This also implies that, no matter how complicated the potential in the interaction area, all its consequences are encoded in this one angle, the so-called scattering angle. This scattering angle may, however, also be influenced by the initial momenta and the masses.

Dropping this condition of elasticity allows to transmute energy and momentum in the potential to an energy loss or gain, a so-called inelastic reaction. Though such a situation can be realized, the system is no longer really closed, as energy and momentum are no longer conserved quantities. In this case, the energy balance is

$$T = T' + Q,$$

where the energy transfer to or from the potential Q can be either negative or positive. Still $\vec{p}'_1 = -\vec{p}'_2$ and the momentum conservation holds trivially in the center-of-mass system. The final state of the system is then no longer entirely determined by the scattering angle θ , but also by Q . Again, both quantities may depend on the properties of the initial state.

While the above describes accurately the situation for the scattering of two particles, it is often useful to make more statistical statements. Especially, it is very often interesting,

how many particles are scattered into which direction per unit of incoming particles. This quantity is called the (differential) cross section and is defined as

$$\sigma(\Omega)d\Omega = \frac{\text{Particles going into } d\Omega}{\text{Total incident particles}}, \quad (2.26)$$

where $d\Omega$ is the solid angle, in three dimensions e. g. $\sin\theta d\theta d\phi$ in the, for this problem particularly suited, spherical coordinates. Integrating the differential cross-section on $d\Omega$ yield the total cross section.

As an example, consider the situation of the gravitational potential of section 2.7.3. Of course, only the non-closed trajectories are interesting, as for the bounded cases no particles are incident or going away⁸. It is useful to define the impact parameter b as the point of closest approach to the center of the potential. It is connected to the angular momentum by

$$l = b\sqrt{2mE} = mv_0b,$$

where v_0 is the speed of the incident particle at infinity. Because of the symmetry of the problem, the scattering, as it is just one of the non-closed trajectories, is in a plane. Thus, by suitably choosing the coordinate frame, there will be no dependence on the angle ϕ , and the cross section will only depend on the azimuth angle θ .

The number of particles N which are then scattered into an azimuth angle of θ are uniquely⁹ determined by the trajectories of section 2.7.3, and thus by their respective impact parameter. In terms of the impact parameters and the number of incident particles equation (2.26) now reads

$$2\pi N b db = -2\pi \sigma N \sin\theta d\theta,$$

where N is the total number of incident particles. This can be rewritten in terms of the cross section, yielding

$$\sigma = -\frac{b}{\sin\theta} \frac{db}{d\theta}.$$

So far, it was not necessary to specify the detailed form of the central potential. Using the form $-\alpha/r$ for the potential yields

$$b(\theta) = \frac{\alpha}{2E} \cot \frac{\theta}{2},$$

⁸Gravitational capture requires thus another, dissipative, effect to reduce the energy of a particle coming from infinity such that it becomes bounded.

⁹This determinism is lacking in quantum physics, where the actual direction of a single particle is given by a probability. Detecting such probabilities belong to the fundamental experiments with which quantum effects have been detected.

and thus

$$\sigma(\theta) = \frac{1}{16} \left(\frac{\alpha}{E} \right)^2 \frac{1}{\sin^4 \frac{\theta}{2}}.$$

This is Rutherford's scattering cross section. Incidentally, the complete quantum calculation for this potential leads to the same result, but this is due to the special structure of the potential, and not true in general.

At first sight, there is one worrisome feature of this result: At small angles, and thus in forward direction, it diverges. This is an artifact of the approximation that the sun (or the gravitational center) only produces the gravitational field, but is otherwise not present. In reality, the particle would collide with the sun, and therefore resolve the structure of it beyond the existence of the gravitational field, and the approximation of a point-like gravity origin breaks down. Of course, deviations will appear already at slightly large than zero angle, because the sun also has a finite extension. Therefore, Rutherford's formula should not be used at small scattering angles. However, it provides a good description at larger angles.

2.8.4 Continuous distribution

So far the situation has been treated that the system is made up of a finite number of individual particles. However, this can actually be generalized to the case where the number of particles becomes infinite, and the system becomes a mass distribution, i. e. a continuous body.

Such a continuous body is characterized by a density $\rho(r)$, a function which determines the amount of mass per unit volume at every point in space. Of course, outside the body this density will be zero. The mass concentrated in some fixed volume V is then given by

$$M_V = \int_V d^3\vec{r} \rho(r).$$

Replacing the finite volume by the whole of space provides the total properties of the body. The quantities from section 2.8.1 can then be readily generalized to yield

$$\begin{aligned} M &= \int d^3\vec{r} \rho(r) \\ \vec{R} &= \int d^3\vec{r} \vec{r} \rho(r) \\ \vec{P} &= \int d^3\vec{r} (d_t \vec{r}) \rho(r), \end{aligned}$$

yielding the total mass, the center of mass and the total momentum of the body, respectively¹⁰. Other quantities are obtained similarly. Most features of continuous mass distributions are therefore just a straightforward generalization of a system of point particles.

2.8.5 Moment of inertia

There is one aspect where the generalization to a mass distribution leads to an interesting new concept.

Consider a body which rotates, but for the sake of simplicity does not translate, around a fixed axis. Furthermore, the axis should be going through the center of mass of the body. In this case the angular velocity is constant and given by $\vec{\omega} = \omega \vec{e}_z$, where the coordinate system has been chosen to be such that the rotation axis coincides with the z -axis.

The speed of rotation at some point \vec{r} inside the body is then given geometrically by

$$d_t \vec{r} = \epsilon_{ijk} \omega_i \vec{r}_j \vec{e}_k,$$

and thus lies entirely in the x - y plane. The total kinetic energy is then given by

$$\begin{aligned} T &= \frac{1}{2} \int d^3 \vec{r} \rho(r) |d_t \vec{r}|^2 = \frac{1}{2} J \omega^2 \\ J &= \int d^3 \vec{r} \rho(\vec{r}) \left| \epsilon_{ijk} \frac{\vec{\omega}_i}{\omega} \vec{r}_j \vec{e}_k \right|^2, \end{aligned} \quad (2.27)$$

where the quantity J is called the moment of inertia. Note that its definition is also valid if the z axis is not the rotation axis.

This moment of inertia is a quantity which characterizes the reaction of a body to a rotation around a given axis. E. g., for a homogeneous cylinder of radius R , height h , and density ρ_0 rotating around its symmetry axis it is

$$J = \int d^3 \vec{r} \rho(r) (x^2 + y^2) = \rho_0 \int_0^R d\rho \int_0^{2\pi} d\phi \int_0^h dz \rho^3 = \rho_0 \frac{2\pi h R^4}{4} = \frac{1}{2} M R^2,$$

where in the last step the mass of the cylinder has been used. For comparison, if the cylinder would rotate around an axis orthogonal through its symmetry axis but going through its center of mass, the moment of inertia would be

$$J = \frac{1}{4} M R^2 + \frac{1}{12} M h^2.$$

¹⁰If the mass distribution would be time-dependent, the last formula needs to be generalized and can be obtained from $d_t \vec{R}$.

Thus, the amount of kinetic energy in the rotation of an extended body is influenced not only by the mass distribution, but also by the relative alignment of the rotation axis with respect to the body.

So far, it was assumed that the rotation axis was going through the center of mass. This will not be the case in general. The consequences of this is described by the theorem of Steiner. In this case, the positions appearing in (2.27) are with respect to the actual rotation axis. Rewriting this position as $\vec{r} = \vec{R} + \vec{s}$, where \vec{R} is the (orthogonal) displacement of the center of mass with respect to the axis of rotation and \vec{s} is the distance to the center of mass. This yields

$$\int d^3\vec{s} \rho(\vec{s}) \left| \epsilon_{ijk} \frac{\vec{\omega}_i}{\omega} (\vec{R} - \vec{s})_j \vec{e}_k \right|^2 = J + \frac{M}{\omega^2} (\vec{\omega} \times \vec{R})^2,$$

where it has been used that

$$|(\vec{R} - \vec{s}) \times \vec{\omega}|^2 = (\vec{R} \times \vec{\omega})^2 + (\vec{s} \times \vec{\omega})^2 - 2 \left((\vec{R}\vec{s})\omega^2 - (\vec{\omega}\vec{s})(\vec{R}\vec{\omega}) \right).$$

The fourth term vanishes since $\vec{R}\vec{\omega} = 0$ by construction. The third term vanishes upon integration, since by construction this is the position of the center of mass for the center of mass being at the displacement position - the vector \vec{s} is measured with respect to the center of mass. I. e. the actual moment of inertia has two components. One describes the rotation of the body as a whole, and the other component the rotation of the body in itself. Thus, again, the two movements separate.

2.9 Perturbation theory

Consider again the one-dimensional case. An interesting situation occurs if a potential $V(x)$ has an extremum at some point x_0 . According to (2.7), the force then vanishes.

Expand now the potential around this minimum in a Taylor series, yielding¹¹

$$V(x) \approx V(x_0) + d_x V(x)|_{x=x_0} (x - x_0) + d_x^2 V(x)|_{x=x_0} (x - x_0)^2 + \mathcal{O}((x - x_0)^3).$$

The first term is just a constant and does not influence the force and hence the motion of the particle. The second term vanishes, since by construction the potential has an extremum. Thus remains the higher-order terms.

In the next step, the situation is considered if the particle is somehow not at x_0 , but rather at some place close to x_0 . If this is the case, $x - x_0$ is small, and all terms in the

¹¹If the potential is non-analytic in x_0 , things become highly non-trivial. This will not be considered for now.

Taylor series becoming increasingly smaller. It is thus possible to consider the particle to only be slightly perturbed, and the movement can be analyzed in perturbation theory, i. e. by discussing the effects of the terms in the Taylor series order by order.

To zeroth order, the potential is constant, and therefore the particle remains at the position x , or moves freely if it has a non-zero initial speed. The next order does not change it, as the second term in the Taylor series vanishes as discussed before.

In the next order, only the quadratic term contributes. But such a potential is just the one of the harmonic oscillator in section 2.6. The resulting movement is known and depends on the sign of $d_x^2 V(x)|_{x=x_0}$. If the sign is positive, the motion of the particle to this order in perturbation theory will be an oscillation around the minimum. Higher orders in the perturbative series will not alter this behavior qualitatively, if just the initial x is close enough to x_0 . Thus in a potential which has a positive second derivative, and thus a minimum, a particle close to the minimum will perform harmonic oscillations around the minimum. Placing it at x_0 without initial velocity will actually leave it at rest, and any small movement outside the minimum will only yield a small oscillation. Thus the equilibrium position x_0 is called stable. Especially, if there should appear any damping of the movement it will be returning to and staying at the equilibrium position eventually.

If the second derivative is actually negative, however, the particle will move, according to section 2.6, exponentially away from the position x_0 . Such an equilibrium position is therefore called unstable. The ultimate fate of the particle is then determined by higher orders in perturbation theory.

There remains the situation if the extremum is actually a saddle point, i. e. the second derivative vanishes. Then again the higher orders will determine the fate of the particle. However, any movement will not be exponential, and therefore the development is much slower. Thus, this situation is called a metastable equilibrium.

Similarly, this implies that a particle which is positioned at the equilibrium position of a potential will react to any infinitesimal external force in one of three ways. If the equilibrium is stable, it will oscillate around it or, if damping is present, return to the equilibrium position. If it is metastable, it will move somewhere, but will eventually be influenced by higher orders of the perturbative series. If it is unstable, it will move away from the equilibrium position.

In this consideration the initial speed has not been an issue. If the speed is so large that the kinetic energy is of a similar size, or larger, than any given order in the perturbative series, the movement is no longer fully described by this order, and higher orders have to be taken into account. If the kinetic energy is small, this will only modify the initial conditions of the movement of the particle to this order. The reason is that the full

potential has possibly not the infinite rising barrier of the harmonic oscillator, but may flatten out. Then the kinetic energy is sufficient to escape this potential well (or feel the distortion away from harmonic), and thus a description to this order of perturbation theory makes no sense.

These concepts can be equally well applied to the situation with multiple extrema. When generalizing to more dimensions, a subtlety arises. In this case, an equilibrium position may have different characteristics in different directions. Then the above said has to be weighted with the direction of the external displacement or perturbation. If the potential is stable/metastable/unstable in this direction, the particle will act accordingly, but may show a different behavior in a different direction.

Besides the possibility to apply perturbation theory for equilibrium positions, perturbation theory can also be used if the potential can be Taylor expanded in a different way. E. g. for the case of two planets around the sun, the gravitational interaction between the two planets is small compared to the sun. Thus with the positions \vec{r}_1, \vec{r}_2 of the two planets and \vec{r}_s of the sun, as well as their respective masses m_1, m_2 , and m_s , it is possible to write the potential for one of the planets as

$$V_1(r) = \gamma \frac{m_1 M_s}{|\vec{r}_1 - \vec{r}_s|} + \mathcal{O}\left(\frac{m_1}{m_s}, \frac{m_2}{m_s}\right),$$

that is, the corrections are small since they are suppressed by powers in m_i/m_s . Thus, the dominating part is a two-body problem, and the remainder can be treated in a perturbative fashion rather accurately. the same is true for the movement of the solar system around the milky way.

2.10 Galileo group

The concept of an inertial system was of central importance in formulating Newton's laws in section 2.2. It is worthwhile to reinvestigating this concept a little more.

The basic starting point is to require that there are coordinate systems in which Newton's first law is valid. Especially, assume that there is one coordinate system in which there are no forces acting on a particle, and it therefore moves with constant speed. If this is the case, then it is possible to define coordinate systems, which are not inertial systems, by having them being accelerated with comparison to the first. There are also other inertial systems, e. g. some which move at constant speed with respect to the first one. In those, also the particle moves at fixed speed.

To systematize this, it is useful to work in the language of linear algebra. Two coordinate systems shall have coordinates \vec{r} and \vec{R} . What will be assumed is that the time in

both frames, t and T , transforms into each other trivially

$$t = T. \quad (2.28)$$

Thus also the time differentials are the same, $dt = dT$. It is this part, which will be lifted when introducing special relativity in chapter 3.

Start with two inertial systems. Then if for a particle of mass m $md_t^2\vec{r} = 0$ is valid, then so must be $md_t\vec{R} = 0$.

Given the path $\vec{R}(t)$ in one coordinate system. In the other coordinate system, it will move as

$$\vec{r}(t) = \vec{r}_0(t) + \Lambda(t)\vec{R}(t),$$

and the difference between both coordinate systems is entirely encoded in the translation $\vec{r}_0(t)$ and the matrix-valued rotation $\Lambda(t)$

$$d_t^2\vec{r}(t) = d_t^2\vec{r}_0(t) + \Lambda(t)d_t^2\vec{R}(t) + 2(d_t\Lambda(t))d_t\vec{R} + (d_t^2\Lambda(t))\vec{R} \quad (2.29)$$

the requirement of both being inertial systems $d_t^2\vec{r} = d_t^2\vec{R} = \vec{0}$ implies $d_t^2\vec{r}_0(t) = 0$, and thus the two coordinate systems cannot be accelerated with respect to each other. Also, this implies that the rotation $\Lambda(t)$ cannot be time-dependent, as otherwise there will be some paths looking like being accelerated. A time-independent rotation, however, is not different from an ordinary rotation of coordinate systems in linear algebra, and will therefore not be considered for now, and hence $\Lambda = 1$.

Thus, up to a rotation, the most general possibility of transformations between two inertial systems is

$$\vec{r}(t) = \vec{v}_0 t + \vec{r}_0 + \vec{R}(t),$$

parametrized by the two vectors \vec{v}_0 and \vec{r}_0 . This is called a Galileo transformation. Note that the forces on a particle are due to (2.2) then identical in all inertial systems, and all coordinate system reachable by Galileo transformations. However, the explicit form may differ, especially if friction is involved.

If two consecutive Galileo transformation are performed, they are equivalent to a single Galileo transformation with

$$\vec{v}_0 = \vec{v}_0^1 + \vec{v}_0^2 \quad (2.30)$$

$$\vec{r}_0 = \vec{r}_0^1 + \vec{r}_0^2. \quad (2.31)$$

and (2.28). Galileo transformations therefore form an (Abelian) group, the so-called Galileo group.

This group can also be extended by including time-independent rotations and reflections. In this case no longer an equality of the forces is true, but the force are still equal up to rotations and reflections.

2.11 Rotating bodies revisited

2.11.1 Pseudo forces

And interesting situation arises when the condition of inertial systems is relaxed. Combining (2.2) and (2.29) yields for a fixed-mass particle

$$\vec{F}(t) = m \left(\Lambda(t) d_t^2 \vec{R}(t) + d_t^2 \vec{r}_0(t) + 2(d_t \Lambda(t)) d_t \vec{R} + (d_t^2 \Lambda(t)) \vec{R} \right). \quad (2.32)$$

The first term is the force in the other coordinate system, up to a (time-dependent) rotation, and therefore the same as with transformations between inertial frames. The three other terms are different.

The first term corresponds to an acceleration of the whole coordinate frame without rotations. It is therefore a relative acceleration. As a consequence, the particle experiences an additional force due to this acceleration. Since this force has no physical origin but emerges just from a an accelerated coordinate system it is not a true force. It is therefore called a pseudo force. Nonetheless, it must be included when describing the movement of the particle inside an accelerated coordinate system. Sometimes these are also called inertial forces.

The other two terms come from a time-dependent rotation of the coordinate systems with respect to each other. They also create pseudo forces. The first term is called the Coriolis force and the second one the centrifugal force. These appear, e. g., when a particle is moving on the surface of a rotating body like the Earth. Though small in this case, they can be measured.

The origin of these forces can also be understood differently. When considering a force-free particle, it will move along a straight line in its inertial system. In an accelerated frame, this path is no longer of constant speed, and may be bend. To describe the effect, this can either be done by the coordinate transformation, or by the forces necessary to modify the path of the particle, which is essentially given by (2.32).

2.11.2 Tensor of inertia

The same approach can be used to discuss the rotation of an extended body at given angular velocity $\omega(t)$. To do so, split the coordinates of every element of the body in two parts. The first part describes the movement of the center of mass of the body, $\vec{R}(t)$, with time-dependent coordinates and time-independent unit vectors. The second vector, $\vec{r}(t)$ represents the movement of any element of the body in the center-of-mass frame, including rotations of the body itself. Thus, \vec{r} is the distance to the center of mass in this coordinate

system. This implies that the unit vectors are time-dependent. The total movement of any element of the body is thus given by

$$\vec{s}(t) = \vec{R}(t) + \vec{r}(t) = R_i(t)\vec{E}_i + r_i\vec{e}_i(t).$$

The speed of any of the points of the body is obtained by a time-derivative, which yields

$$d_t\vec{s}(t) = d_tR_i(t)\vec{E}_i + r_id_t\vec{e}_i(t) = d_t\vec{R}(t) + \vec{\omega}(t) \times \vec{r}(t)$$

since the time change of the unit vectors describing the body is just the angular velocity.

This result is a prototypical one. It describes that the a time derivative is split into two components,

$$d_t = d_t^R + \omega \times,$$

i. e. the time derivative acting on the total movement is a composition of two elements. One describes the action on the center of mass, and another one relative motion to it. This may seem to be rather strange at first, but the generalization of this so-called operator identity plays a very crucial role throughout physics, especially in general relativity and particle physics. It shows how changes split into outer and inner components. It is thus also called a covariant derivative.

This view leads to a generalization of the moment of inertia of section 2.8.5. The total kinetic energy is

$$T = \frac{1}{2} \int d\vec{r}^3 \rho(\vec{r}) (d_t\vec{s})^2 = \frac{1}{2} \int d\vec{r}^3 \rho(\vec{r}) \left((d_t\vec{R})^2 + (\vec{\omega} \times \vec{r})^2 + 2(\vec{\omega} \times \vec{r}) d_t\vec{R} \right).$$

The first term is the kinetic energy due to the center-of-mass movement.

The third term is only relevant if the center of mass does not move. However, by construction

$$(d_t\vec{R}) \left(\vec{\omega} \times \int d\vec{r}^3 \rho(\vec{r}) \vec{r} \right) = 0,$$

since the integral is proportional to the center of mass in the center-of-mass frame in which \vec{r} is measured, and therefore by construction zero. Thus, the third term never contributes.

Note that

$$(\vec{\omega} \times \vec{r})^2 = \vec{r}^2 \vec{\omega}^2 - (\vec{r} \vec{\omega})^2 = r_i^2 \omega_j^2 - (r_i \omega_i)^2 = (\vec{r}^2 \delta_{ij} - r_i r_j) \omega_i \omega_j$$

and it is thus possible to split the expression into a product depending only on the body and one only on the rotation. This is a matrix-vector product. Hence, this is used to define the (symmetric) tensor of inertia¹²

$$J_{ij} = \int d\vec{r}^3 \rho(\vec{r}) (\vec{r}^2 \delta_{ij} - r_i r_j).$$

¹²The name tensor is justified, as it can be shown that the so-defined matrix indeed transforms in the prescribed way as a second-rank tensor.

The kinetic energy is then given by

$$T = \frac{1}{2}M(d_t\vec{R})^2 + \frac{1}{2}\vec{\omega}^T J \vec{\omega},$$

and the splitting between translation and internal rotation becomes manifest again.

Since the tensor of inertia is symmetric, it can be diagonalized, having its eigenvalues on the diagonal. These eigenvalues describe the moments of inertia around rotations along the respective axes in this system, which are the main axes of the body in question. If the body is an ellipsoid, these are just the usual three main axes of this ellipsoid.

This tensor of inertia is also determining the angular momentum of the total movement, \vec{l}_s as a straightforward and analogous calculation shows,

$$\vec{l}_s = M\vec{R} \times d_t\vec{R} + J\vec{\omega} = \vec{L} + \vec{l}. \quad (2.33)$$

Thus, it is also possible to rewrite the kinetic energy as

$$T = \frac{1}{2}M(d_t\vec{R})^2 + \frac{1}{2}\vec{\omega}^T \vec{l},$$

and thus as a combination of the motion of the center-of-mass and the rotation of the body.

Chapter 3

Special relativity

So far, classical mechanics was essentially describe by Newton's laws of section 2.2, supplemented with forces. Both together form as postulates the framework of classical mechanics. However, it turns out that classical mechanics based on these postulates is not able to describe all situations, no matter how complicated the forces are assumed to be. Of course, also electromagnetic, including optical, phenomena are not described by classical mechanics. However, supplementing Newton's laws with Maxwell' laws this is possible, but does not lead to anything conceptually new on the sides of mechanics, as those cases to be discussed here do. Note that thermodynamics and hydrodynamics are actually only the application of classical mechanics to large ensembles of particles, and therefore do not require fundamentally new laws, as can be shown using statistical (classical) mechanics.

The situations where failures arise are, together with their resolutions or combinations of resolutions,

1. At very short distances. This is the purview of quantum mechanics
2. High speeds. This is the purview of special relativity
3. Strong gravitational fields. This is the purview of general relativity, which necessarily induces large speeds and thus includes special relativity
4. at short distances and high speeds. This requires the combination of quantum mechanics and special relativity, which becomes quantum field theory. Note that a full inclusion of electrodynamics in quantum mechanics requires quantum field theory
5. at all of the above. This requires the combination of quantum physics and general relativity is the, not yet fully formulated, quantum gravity

Besides electrodynamics and gravity, there are also two more known sources of forces, the weak and strong nuclear forces. All known forces can actually be derived from these four, though a unifying theory of all of them is not yet available.

Relaxing all of these conditions, and covering everything listed, essentially sums up the complete master study of (theoretical) physics. As a first step, here one of those will be included, those which is the least complicated one: Special relativity, i. e. the modifications necessary to classical mechanics when including large speeds.

3.1 The speed of light and Minkowski space

3.1.1 The equivalence principle

The starting point of special relativity is a reevaluation of Galileo's transformations of section 2.10. Consider a system which moves with a constant speed with respect to another one. This implies that the coordinates in one system are related to the other by

$$\vec{r}' = \vec{r} + \vec{v}t,$$

where \vec{v} is the relative speed of the two systems. These are inertial systems, and thus Newton's laws hold equally in both of them. But speeds measured in one system differ by speeds in the other system, since

$$d_t \vec{r}' = d_t \vec{r} + \vec{v}. \quad (3.1)$$

This should be a true statement for any moving object when described in either coordinate system.

This is where a contradiction to experiments arises. While the relation (3.1) holds to very good accuracy experimentally at low speeds, it does not do so at large speeds. In fact, the deviation is there also at low speeds, but it becomes quickly so tiny, as will be quantified later, that it is below any reasonable experimental uncertainties if the speed is just low enough. Thus, something does not fit.

As it turns out, Newton's postulate are the problem. More precisely, their statements about inertial systems and that Newton's second law (2.2) holds equally in all inertial systems connected by Galileo transformations. The reason is that Newton's laws make a very deep assumption about space-time: That space-time has an Euclidean structure. However, as it turns out, nature is not of this form, but has a more complex structure, which only at low speeds looks Euclidean.

In principle, the only necessary thing is to replace the space-time structure accordingly, and then derive the results from this.

It is, however, more instructive, to pursue a slightly different path, where the space-time structure stands at the end. As always, there are several equivalent ways of formulating the basic postulates, and each form implies the other.

This different approach will start rather from a physics motivation.

Consider again Newton's laws. It may look like that the second law, equation (2.2), is the most important part. Just because so far this was the one made most reference to. But this is not quite the case. The probably most important statement is that physics is the same in all inertial systems. As the choice of inertial system is done by an observer, this implies that physics is independent of any observer. While this appears obvious at first, this is actually a very deep statement. And a postulate. Changing (2.2) somewhat would just change the resulting trajectories. Changing this statement would give up any notion (or even hope) of something like an objective reality¹.

So, this will be the first part of the new set of postulates: Physics is observer independent. This implies that the further postulates should have the same form in every inertial frame. In particular, this implies it is impossible to make statements about the frame from within the frame: There is no absolute frame. Only relative differences between frames can be identified. This is known as the equivalence principle.

So far, this seems not be something different than Newton's requirement that physics should be the same in all inertial frames.

The big difference comes from an experimental observation: All massless particles move at a fixed speed. It is called the speed of light c , as light in the form of photons has been the first observed particles to be massless. Since this speed must therefore be the same in all frames, this implies that (3.1) cannot be correct. Or more aptly put: Galileo transformations are not appropriate to transform between frames. Since this transformation comes from the assumption of an Euclidean space-time, it is this assumption, which must be wrong. It now remains to work out the consequences. This is entirely based on the equivalence principle and the experimental observation of a unique speed of massless particles in every frame². That massless particles may create a problem can also be seen from Newton's law (2.2), as it implies that massless particles cannot be described by it. Though this can be alleviated by the formulation using (2.1), it still leaves a certain feeling of uneasiness. Also this will be fixed in special relativity.

¹Whether such a thing can exist at all is an unsolved question of science philosophy. In physics, it is the description of observations, which is the core duty. And so far all observations available very uniquely point to an observer-independent description.

²Historically, it was not the speed of massless particles, but of the speed of light. However, this would require electrodynamics, which will be avoided here, as considering massless particles lead to the same result

3.1.2 Minkowski space

So, it is now clear that something is not right with the way inertial frames, and transformations between, are defined. This leads to the question how this can be fixed. Consider the distance traveled by a massless particle with its fixed speed³ c . In a given reference frame, the distance traversed in time t will be

$$\vec{r}^2 = c^2 t^2.$$

Something which would be nice to keep is that space is isotropic - the x , y , and z directions are all the same. The question is, how does this change to a new coordinate system. There are several possibilities. E. g., the left-hand side could change by changing the metric, additional terms could arise, and many more. Experiment would have to decide, which is correct. Though instructive, considering all possibilities would lead far beyond the scope of this lecture. Therefore, with hindsight, the only change will be to give t a non-trivial transformation property, i. e. the time could also differ in both coordinate systems. This deviates from the starting point of the Galileo transformation (2.28).

In another coordinate system then the relation

$$\vec{r}'^2 = c^2 t'^2$$

holds, where the important piece is that c is the same in both equations. Since zero is zero, both equations can be combined to yield the equality

$$\vec{r}^2 - c^2 t^2 = \vec{r}'^2 - c^2 t'^2. \quad (3.2)$$

In the case of a Galileo transformation, a similar equality holds, but there c would be transformed and t would be fixed.

Nonetheless, such a relation as (3.2) looks quite familiar from linear algebra. It reminds of an invariant length, but of a vector space with a non-Euclidean metric. This is actually correctly inferred.

Define now space-time as a vector space, the so-called Minkowski space, \mathbb{M}^4 as a vector space having a non-trivial metric⁴

$$g^{\mu\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

³Which is, of course, the speed of light.

⁴It is equivalently possible to switch the signs of all entries, $g \rightarrow -g$, without changing the physics. This will be discussed more in detail below, and is thus a convention.

Then this defines a four-vector⁵

$$x = \begin{pmatrix} ct \\ \vec{x} \end{pmatrix} = \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix}.$$

Conventionally, the components of this vector are enumerated with Greek literals starting from zero, $x_0 = ct$, $x_i = (\vec{x})_i$, while the Latin indices still enumerate the spatial components starting at 1.

The scalar product is then

$$x^2 = x^T x = x_\mu g^{\mu\nu} x_\nu = -(ct)(ct) + (\vec{r})(\vec{r}) = \vec{r}^2 - c^2 t^2,$$

and thus in such a space indeed (3.2) is a preserved length. The question is now, whether the standard linear algebra for such a space correctly reproduces physics. Most interesting is, of course, whether rotations in such a space are compatible with the equivalence principle and the speed of light.

As it will turn out that this is indeed correct, it is useful to repeat a few results about vector spaces with non-Euclidean metric. Since it has been the question of coordinate transformations which led to this point, the first important step is that of how they work in Minkowski space.

First of all, a translation works as usual, i. e. a replacement $x_\mu \rightarrow x_\mu + a_\mu$ shifts the origin. The only difference is that, in contrast to the Galileo transformations of section 2.10 a_0 also automatically shifts the origin of time.

Leaves rotations. Here it is once more important to remind of the concept of tensors. Rotations are matrix-valued operations U , which leave the scalar product invariant, in Euclidean spaces

$$\vec{x}^T \Lambda^{-1} \Lambda \vec{x} = \vec{x}^T \vec{x}.$$

However, this is true, no matter whether \vec{x} goes to $\Lambda \vec{x}$, as above, or $\Lambda^{-1} \vec{x}$. This gives rise to define covariant and contravariant tensors.

Given that the coordinates transform as

$$\Lambda x,$$

⁵In older texts this is often done by having an ordinary Euclidean metric but making the time component (or all space-components) purely imaginary. While for special relativity this does not make any difference, this is not well suited for generalizations, which are quite interesting nowadays. It will therefore not be used here.

any object which transforms in the same way is called a covariant tensor (of rank 1). Any object transforming like

$$\Lambda^{-1}x$$

is called a contravariant tensor (of rank 1). To separate both quantities, covariant tensors will have their index down, x_μ , and contravariant tensors up x^μ . Likewise, it will be defined that the transformation matrix Λ has its indices mixed, and

$$\Lambda^\mu_\nu = (\Lambda^{-1})^\nu_\mu. \quad (3.3)$$

Thus, the transformation rules read

$$\begin{aligned} (x')_\mu &= \Lambda^\nu_\mu x_\nu \\ (x')^\mu &= \Lambda^\mu_\nu x^\nu, \end{aligned}$$

that is the doubly appearing, and thus summed, indices are appearing once up and once down.

Tensors of higher rank are then defined by their transformation properties on their indices. If it transforms by a product of Λ , it is called a covariant tensor,

$$(M')_{\mu_1 \dots \mu_n} = \Lambda_{\mu_1}^{\nu_1} \dots \Lambda_{\mu_n}^{\nu_n} M_{\nu_1 \dots \nu_n},$$

of rank n and

$$(M')^{\mu_1 \dots \mu_n} = \Lambda_{\nu_1}^{\mu_1} \dots \Lambda_{\nu_n}^{\mu_n} M^{\nu_1 \dots \nu_n},$$

a contravariant tensor of rank n . If some mixtures of Λ and Λ^{-1} appear, it is called a mixed tensor.

What has not yet been defined is how the transformation matrices Λ should look like, such that (3.2) is correct. This will happen if

$$v^{T'} w' = v^T \Lambda^T g \Lambda w = v^T w$$

is satisfied. Note that this implies

$$\Lambda^T g \Lambda = g, \quad (3.4)$$

and thus the Λ must leave the metric g invariant.

It turns out that there are six basic matrices satisfying the condition (3.4),

$$\begin{aligned}
 J_1 &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \alpha & \sin \alpha & 0 \\ 0 & -\sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}; & J_2 &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \beta & 0 & \sin \beta \\ 0 & 0 & 1 & 0 \\ 0 & -\sin \beta & 0 & \cos \beta \end{pmatrix}; & J_3 &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos \gamma & \sin \gamma \\ 0 & 0 & -\sin \gamma & \cos \gamma \end{pmatrix} \\
 J_4 &= \begin{pmatrix} \cosh \eta & \sinh \eta & 0 & 0 \\ \sinh \eta & \cosh \eta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}; & J_5 &= \begin{pmatrix} \cosh \xi & 0 & \sinh \xi & 0 \\ 0 & 1 & 0 & 0 \\ \sinh \xi & 0 & \cosh \xi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}; & J_6 &= \begin{pmatrix} \cosh \zeta & 0 & 0 & \sinh \zeta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \sinh \zeta & 0 & 0 & \cosh \zeta \end{pmatrix}.
 \end{aligned} \tag{3.5}$$

all other matrices satisfying the condition (3.4) can be written as a product of these six elementary matrices. The first three can be recognized as rotations in three-dimensional space, when ignoring the time. This is not surprising, as the spatial components of the metric g are just an ordinary Euclidean metric, and any invariance there will simply require that the transformation matrices Λ are rotation matrices. The other three are odd. But before continuing with them it is useful to derive some more general statements.

Note first that

$$\Lambda^{-1}\Lambda^T = 1$$

for the matrices J_1 to J_3 , since $\Lambda^T = \Lambda$ for them. For the other three $\Lambda^{-1} = \Lambda^T$, as for ordinary rotations. From this follows that, depending if Λ is constructed from the first or the second three⁶

$$\begin{aligned}
 \Lambda^{-1}gv &= \Lambda^{-1}g\Lambda^{-1}\Lambda v = \Lambda^T g \Lambda \Lambda v = gv' \\
 \Lambda^{-1}gv &= \Lambda^{T-1}g\Lambda^{-1}\Lambda v = (\Lambda^{-1})^T g (\Lambda^{-1})\Lambda v = gv',
 \end{aligned}$$

where the first line applies to ordinary rotation and the second one to the new class of matrices. But this implies that gv transforms like a contravariant tensor. It is therefore said that g raises an index, as

$$g^{\mu\nu}v_\nu = v^\mu.$$

Thus, a contravariant vector differs from its covariant version by a minus sign in the first component. It can likewise be shown that a matrix with entries defined as solutions to

$$g_{\mu\nu} = g^{\mu\rho}g^{\nu\sigma}g_{\rho\sigma}$$

⁶Mixtures can be deconstructed as consecutive transformations.

has the effect that

$$g_{\mu\nu}v^\nu = v_\mu$$

reverses the change from contravariant to covariant, and furthermore

$$g_{\mu\nu}g^{\nu\rho} = \delta_\mu^\rho,$$

and can be thought of the inverse of the metric. This also implies that a scalar product is

$$v_\mu g^{\mu\nu} v_\nu = v_\mu v^\mu,$$

and therefore equivalent to the product, without metric, of a covariant and a contravariant vector.

The consequence of such a metric is that scalar products are no longer positive semi-definite. Especially

$$v^T g w = a$$

can now be greater, smaller or equal zero, even if $v = w$. Thus, vectors can be classified by the fact whether they have positive, negative, or zero length. Examples for all possibilities in two dimensions are

$$\begin{aligned} v_1 &= \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \\ v_2 &= \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \\ v_3 &= \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \end{aligned}$$

where these vectors have negative, zero, and positive norm, respectively. Vectors with negative norm are called timelike, vectors with zero norm are called lightlike, and vectors with positive norm are called spacelike, for reason to be come clearer later.

This also implies that the 'angle'

$$\frac{v^\mu w_\mu}{|v||w|}$$

between two vectors needs no longer to be a real angle, and in fact this expression needs no longer to vary between -1 and 1, as it does in Euclidean metric. Rather, as with rotations before, this should be considered to be a generalized angle η , and this expression equal to $\cosh \eta$.

Note that nothing of these changes when multiplying the starting point (3.2) by a minus sign, except that the necessary metric would have reversed signs. Thus, this is equivalent, a matter of convention, whether the negative or the positive norm is conserved. However, this will reverse also the signs for the classification of timelike and spacelike. Thus care should be taken to stick with a single convention.

This leaves to understand the transformations induced by J_4 to J_6 . Applying it to a vector delivers, say,

$$J_4 x = \begin{pmatrix} ct \cosh \eta + x \sinh \eta \\ x \cosh \eta + ct \sinh \eta \\ y \\ z \end{pmatrix},$$

and likewise J_5 and J_6 . I. e. they mix spatial positions and time, which is very different from ordinary rotations.

It remains to determine how η , ξ , and ζ are related to the parameters of the transformation. Consider two coordinate systems moving relative to each other at a fixed speed v along the x -axis. The origin of the new coordinate system must satisfy

$$vt \cosh \eta + ct \sinh \eta = 0$$

as the two move with respect to each other. Using

$$\cosh \eta = \sqrt{1 + \sinh^2 \eta},$$

the solution for $\sinh \eta$ is

$$\begin{aligned} \sinh \eta &= \frac{\frac{v}{c}}{\sqrt{1 - \frac{v^2}{c^2}}} = \gamma \beta \\ \beta &= \frac{v}{c} \\ \gamma &= \frac{1}{\sqrt{1 - \beta^2}}. \end{aligned} \tag{3.6}$$

This leads finally to the Lorentz transformations

$$J_4 x = \begin{pmatrix} \gamma(ct - \beta x) \\ \gamma(x - \beta ct) \\ y \\ z \end{pmatrix}. \tag{3.7}$$

If the speed is small, $\beta \approx 0$ but $c\beta = v$, this reduces to

$$J_4 x \stackrel{\beta \approx 0}{=} \begin{pmatrix} ct \\ x - vt \\ y \\ z \end{pmatrix},$$

and therefore reduces to the Galileo transformation, in accordance with the requirement that at low speeds conventional Newtonian physics should reemerge.

The matrices J_i therefore define the possible norm-conserving transformations. The J_{1-3} are ordinary rotations, and the J_{4-6} describe movements along the three coordinate axes with constant velocities, so-called boosts. Both together form the so-called Lorentz group, in analogy to the conventional rotation group, which is sometimes abbreviated to $SO(1,3)$.

However, all of this is essentially only replacing the arena of mechanics. It is not yet defined how the dynamics, and even the kinematics, should be formulated. This will be done in the following.

It should be noted that a shift by a constant (four) vector is satisfying all the above criteria, and is still an admissible transformation. Combining the above Lorentz transformation, the so-called proper Lorentz transformations, with these translation leads to the so-called Poincare transformations. They can be supplemented by operations like space and/or time inversions.

3.2 Measurements of time and distance

To define the kinematics requires to give meaning to distances and time differences, to ultimately define speeds and accelerations. This requires to understand how distances are perceived in different coordinate systems.

To understand why this is not obvious, note that in (3.7) not only space changes, but also time. Especially, in relatively boosted systems two events will not take place at the same time - concurrence as known in the Galileo group is lost.

Consider now some rigid object with an extension $l = x_2 - x_1$ in its rest frame. An observer moving along the x -axis will define in her frame of reference the length of the stick by the difference in endpoints at the same time in her coordinate system. As noted, this does not correspond to the same time in the original coordinate system. It is thus best to use the inverse of (3.7), since

$$x_i = \gamma(x'_i + \beta ct')$$

Calculating the difference yields

$$l' = x'_2 - x'_1 = \gamma^{-1}x_2 - \beta ct' - \gamma^{-1}x_1 + \beta ct' = \gamma^{-1}l.$$

Thus, the stick is shorter in the moving frame, as γ^{-1} is always smaller than 1. This has nothing to do with the finiteness of a maximal speed: Using a Galileo transformation and a finite speed to transfer the information from the different points of the beginning and ending of the stick will yield a different result. The reason is that spatial distances, due to (3.2), are shorter - a Lorentz transformation only preserves the length element (3.2), but not a spatial length element. That this leads to actual shorter distances is because of the minus sign in the metric. This phenomena is called length contraction.

In the same way time differences measured at the same point change, and become

$$\Delta t' = t'_2 - t'_1 = \gamma(t_2 - t_1) = \gamma\Delta t,$$

but they appear longer. The reason for this is the opposite sign of spatial and temporal parts of the metric. This phenomena is called time dilatation.

It is important to note that this is a reflexive phenomenon: Not only will the observer in the moving frame think sticks are shorter and times longer in the other frame, an observer in the other frame will see the same for the primed frame. This is the equivalence principle at work. In both frames, physics looks the same, as it is not possible to have an absolute speed, merely a relative speed⁷.

In the end, both time dilatation and length contraction should not come as a surprise. Lorentz transformations only keep the norm of a 4 vector invariant. Both spatial length and time are only components of a 4 vector. Therefore, they are not separately invariant. This is as for ordinary rotations in Euclidean space: Performing a rotation, the components of a vector are not individually invariant, but only the total length. And just like as with rotation, and reduction in one component's absolute value has to be compensated by an increase in another component's, and thus also some opposite effect has to be expected for both time and space here. Although the indefinite norm has some influence on this naive picture.

Another interesting feature is what happens when performing two boosts after each other. This makes statements about how speeds add to each other. Multiplying, say, J_4 twice for two different speeds, yields

$$J_4(\eta)J_4(\xi) = J_4(\eta + \xi) = J_4(\zeta),$$

⁷Note that these are statements only in frames moving with fixed speed to each other. Accelerated frames, e. g. when starting at the same point, but one accelerated and then coming back at some point in the future, need general relativity to accurately describe.

which uses that

$$\begin{aligned}\cosh(\eta) \cosh(\xi) + \sinh(\eta) \sinh(\xi) &= \cosh(\eta + \xi) \\ \cosh(\eta) \sinh(\xi) + \sinh(\eta) \cosh(\xi) &= \sinh(\eta + \xi),\end{aligned}$$

which shows that expressed in these quantities boosts are additive. Using (3.6), this implies for the total β value

$$\beta = \frac{\beta_1 + \beta_2}{1 + \beta_1 \beta_2} \stackrel{\beta_i \leq 1}{=} \beta_1 + \beta_2$$

This so-called Einstein's addition theorem of velocities has a number of remarkable properties. First, at small speeds it reduces to its Galileo form (2.31), and once more shows how Galileo transformations emerge as a limiting case of Lorentz transformations. The second is that this implies that the total speed can never exceed the speed of light, as for any values of $\beta_i \leq 1$ the total speed also satisfies $\beta \leq 1$. In fact, if both speeds are at the speed of light, the total speed is also the speed of light. This implements the experimental observation that there is no speed possible faster than the speed of light. In fact, the only solutions for $\beta > 1$ require the β_i to be complex, a physical not sensible result.

This observation has far-reaching implications. The probably most profound is that there are events, i. e. points localized in space and time, which cannot influence each other. This is because their distance is so large that no object can reach them quickly enough. They are said to be causally disconnected. In a fixed coordinate system, this happens as two points cannot communicate earlier than a signal traveling at the speed of light can travel from one to the other⁸.

This happens, if

$$(ct)^2 < (\vec{r})^2.$$

But this is nothing than the statement that the connecting vector of both events has a positive norm. Thus, this justifies the name spacelike for these vectors, as there is always an intervening space. On the other hand, two events can interfere if the opposite holds, and thus the connecting vector is timelike. Finally, the borderline is the case of zero length, and thus lightlike vectors. As the length of the vectors are invariant under a Lorentz transformation, by construction, causal connections remain invariant under the change of coordinate systems, as it must be, since causal influence is a physical feature, and thus must be the same in all frames.

This fact can be visualized by the so-called light-cone, which is the part of Minkowski space, for any fixed point, which has a timelike distance to the reference point. All points

⁸In a more refined version, it is actually that no information, carried by energy, can be transported faster than the speed of light. While in principle more exact, this will make only a difference when introducing fields.

in the past to the event can therefore causally influence it, will the event itself can causally influence any event in its future light-cone, where past is defined by $t < t_0$ and future by $t > t_0$, where t_0 is the time coordinate of the event. Also these light-cones are invariant under Lorentz transformations, and the same in all frames.

3.3 Relativistic kinematics

With this all necessary ingredients are available to describe the motion of a particle in special relativity, and thus relativistic kinematics and, ultimately, dynamics.

To achieve this aim, it is best to be inspired by the classical case and how it reacted to rotations. The basic ingredient in the formulation of Newton's laws was to require the involved quantities to be vectors. To achieve that physics is invariant under rotations was to formulate all equations in terms of tensors of the same type on the left-hand side and the right-hand side. Thus, Newton's law (2.2) is actually an equation involving two tensors of the same rank, both being actually Euclidean covariant tensors of rank 1.

In the same way, the generalization will be completely in agreement with Lorentz invariance - often called covariant - if particular care is taken to involve only tensors of the same rank and type on both sides of the equations.

The first task is to describe the trajectory of a particle. It is given by a sequence of four-vectors x . So far, the position along the trajectory has been identified by the time. This was possible, as time was an immutable concept. Now, however, time is itself part of the trajectory. It is therefore no longer a suitable concept, and a new trajectory parameter seems more appropriate, which uniquely identifies a position along the trajectory.

To find one, consider an infinitesimal move along the trajectory. The length of this move is given by

$$\frac{1}{c^2}(dx_\mu)^2 = -(d\tau)^2$$

where the prefactor is chosen by convention. The right-hand side now defines a quantity τ , which is called the eigenzeit, and which by construction exactly describes the change in trajectory, as the advance is uniform in it. It should be noted that the trajectory $x_\mu(\tau)$ is also called a world-line, as it describes the propagation of a particle along a line in the space-time world.

When changing to the rest frame, this reduces to

$$(d\tau)^2 = -\frac{1}{c^2}(dx_\mu)^2 = \frac{1}{c^2}(dct)^2 = (dt)^2.$$

Thus, in the rest frame, sometimes also called eigenframe, the eigentime is the ordinary time, justifying its name and its normalization. Note that by convention the eigenzeit is

taken to be the positive value. Note further that for any arbitrary frame

$$d\tau = \sqrt{\frac{1}{c^2} ((dct)^2 - (d\vec{r})^2)} = dt \sqrt{1 - \frac{1}{c^2} \left(\frac{d\vec{r}}{dt} \right)^2} = \gamma^{-1} dt$$

Thus, the time interval dt is the one measured in a system moving with respect to the particle's restframe. This again makes the eigen part of the name *eigenzeit* clearer: τ is the time in the restframe of the particle, which is used to describe its trajectory.

The *eigenzeit* can now be used to generalize the concept of speed to the four velocity

$$u_\mu = \frac{dx_\mu}{d\tau} = \gamma \frac{dx_\mu}{dt} = \begin{pmatrix} \gamma c \\ \gamma \vec{v} \end{pmatrix} \stackrel{\beta_i \ll 1}{\approx} \begin{pmatrix} c \\ \vec{v} \end{pmatrix}. \quad (3.8)$$

The last equality shows why this is a useful generalization of the concept of speed, as it reduces at low speed to the conventional one.

It is an interesting feature that the length of the four speed is actually constant,

$$u_\mu u^\mu = \gamma^2 (\vec{v}^2 - c^2) = -c^2 \frac{1 - \beta^2}{1 - \beta^2} = -c^2.$$

Note that this is also true at low speeds, as then \vec{v}^2 can be neglected compared to c^2 on the right-hand side. This also implies that the four-speed is a timelike vector.

3.4 Relativistic version of Newton's laws

To formulate a relativistic generalization of (2.2), the first postulate is that the mass of a particle, m , is still a well-defined quantity, and especially does not change under Lorentz transformations.

To generalize Newton's law, it is best to start from the more general formulation using the momentum, (2.1). The relativistic momentum is given by $p_\mu = m u_\mu$, as a direct generalization of the non-relativistic one, and which, due to (3.8), reduces to the non-relativistic one at low speeds.

It then remains to postulate the relativistic version of Newton's law such that it is an equation in terms of four-vectors. This is

$$\frac{dp_\mu}{d\tau} = K_\mu = \begin{pmatrix} \gamma \vec{\beta} \vec{F} \\ \gamma \vec{F} \end{pmatrix} \stackrel{\beta_i \ll 1}{\approx} \begin{pmatrix} \vec{\beta} \vec{F} \\ \vec{F} \end{pmatrix}. \quad (3.9)$$

By construction, this has the correct low-speed limit.

However, the fourth component of (3.9) looks strange, and requires further scrutiny. Going back to conservative forces in (2.12),

$$d_t T = \vec{F} \vec{v}.$$

Thus, the fourth component of (3.9) is associated to the change of kinetic energy in the non-relativistic limit. Conversely, this implies that

$$T = \gamma m c^2 \stackrel{\beta_i \ll 1}{\approx} m c^2 + \frac{m \vec{v}^2}{2} \quad (3.10)$$

is the relativistic generalization of the kinetic energy. In particular, this kinetic energy is conserved in the absence of forces. Thus, the fourth component of the four momentum is the kinetic energy.

There is however still the question of the constant in (3.10). It seems to make no sense that a particle at rest has kinetic energy. The reason is that it should rather be interpreted as the total energy of the particle, and this is a contribution to this total energy every particle has, even at rest. As this kinetic energy is proportional to the mass, this is also called the rest energy of the particle. It is therefore useful to reinterpret it as the total energy of a particle E .

From this follows

$$p_\mu p^\mu = -m^2 c^2 = \vec{p}^2 - \frac{E^2}{c^2}$$

or that the energy of a relativistic particle is given by

$$E = \sqrt{\vec{p}^2 c^2 + m^2 c^4} \stackrel{\vec{v}=\vec{0}}{=} m c^2, \quad (3.11)$$

giving a connection between energy and mass. This is a very important statement, as it implies the equivalence of energy and mass, and therefore the possibility to convert one into the other: Mass is no longer a conserved quantity, even if it is a scalar quantity. It can be transformed to energy, which then again can be conserved to mass, thereby changing the identity of particles.

What remains in place is Newton's third law of action and reaction. An important consequence of this is

$$d_t p^1 + d_t p^2 = K^1 + K^2 = K^1 - K^1 = 0.$$

Thus, the total four momentum is conserved in a closed system. This also implies that energy is conserved, as this statement holds component-by-component. Four-momentum conservation supersedes energy and momentum conservation of non-relativistic mechanics. This is especially different, as here only the energy is conserved, but this does not need to

be in form of mass. Rest mass is no longer individually conserved, but only accidentally, if four momentum conservation implies it. That is of particular importance for the relativistic generalization of scattering processes.

It should also be noted that (3.9) no longer implies that the acceleration \vec{a} needs to be proportional to the force, as it also contributes to the fourth component. As a consequence, a particle can experience lateral accelerations with respect to the force. Such effects can be measured, and represent a genuine effect entirely due to special relativity.

Note finally that a free particle will again have a constant four-velocity, and thus move along a straight line in the three-dimensional subspace.

So far, still the mass appeared throughout, and it is not yet clear, how massless particles should act. However, (3.11) implies for massless particles

$$E = c|\vec{p}|,$$

and thus for a massless particle the momentum is proportional to the energy. Moreover, (3.11) shows that in the massless case the four-momentum becomes light-like rather than space-like. This implies that it describes a movement of a particle at the speed of light, rather than that of a massive particle with a finite speed.

While the formulation (3.9) is certainly a possible formulation of relativistic dynamics, it is actually not a very convenient one. It is therefore useful to first introduce a particular formulation of classical mechanics, in which special relativity can be more easily embedded.

In addition, there is a conceptual problem in applying (3.9). Considering forces like the one of a harmonic oscillator or the gravitational force, they entail the problem that these forces act everywhere simultaneously. It is certainly possible to use the one-particle version in (3.9), as this corresponds to an eternal and immutable force field, which does not change over time. But the situation becomes more complicated when considering the two-body problem with the original gravitational force (2.3). It uses the positions of every particle at a given instance of time. Thus, it assumes that the information about the propagation of a particle is instantaneously transmitted to the other particle, and vice versa. This is inconsistent, as the maximum speed in special relativity is the speed of light. Thus, though it is formally possible to use this force in (3.9), the results will not be compatible with physics. Rather, the force itself needs to have the speed of light as maximum propagation speed build in. Thus, treating dynamical problems is far less trivial, as it requires also new postulates for the forces. To attack this problem also a different formulation is better suited, which starts from scratch from covariant quantities.

Thus, now the corresponding formulations will be developed in classical physics, and their fully special relativistic form then discussed in section 5.6.

Chapter 4

Lagrangian mechanics

In the previous chapters the basic concepts of mechanics have been formulated. All of the basic physical mechanisms have been collected. The only thing in which other problems of mechanics would differ is by other versions of the forces or, if existing, potentials. All the conceptual ideas are there.

The following chapters do not aim at any more elaborate problems with more complicated potentials and/or systems until chapter 6.

Rather, this and the next chapter 5 aim at a reformulating of mechanics. While this provides at first sight no new physical systems, this will emphasize concepts which act on a more fundamental level. Furthermore, these two chapters provide the basis for the generalization of mechanics to quantum mechanics. Finally, in more complicated situations the methods to be discussed in the following turn out to be superior to the ones introduced so far.

The downside of this is that the motivation for many of the ideas in the following is not at all obvious at first. In fact, without dealing either with much more complex problems or with quantum physics most of the following will be rather experienced as a complication rather than a simplification. However, would one introduce the following with suitable complicated problems, the sheer complexity of the problems would overlay everything, and therefore the formalism would become obscure. It is therefore a precarious problem to exhibit the reason behind this formalism.

4.1 Constraints

The first basic insight is the realization that most particle movements are not as simply described as before.

Consider, e. g., a particle moving through a winding tube under the influence of gravity.

The particle cannot move in all directions equally, but is confined to a one-dimensional path through the tube. To have such a path requires that the walls of the tube acts with a force on the particle, on top of the gravitational force. Otherwise the particle would fall through the tube walls, following the pull of gravity. To describe this using Newton's equation (2.2) would require to know the particularities of these forces, which are so-called constraining forces. In general these constraining forces are essentially impossible to determine, which appears to make the solution of the problem using the techniques of chapter 2 essentially impossible.

The necessary insight to deal with this problem is that it is actually not necessary to really know these forces in detail, since the consequences of them are known: The particle remains in the tube. The consequence of that is that the three coordinates, x , y , and z , are no longer independent. Since the particle moves along the tube, there is only one way to go (either forward or backward). So, effectively its movement is reduced to one dimension. Hence two of the coordinates are actually functions of the third, e. g. $x(z)$ and $y(z)$.

Of course, the choice of z was arbitrary. Therefore, it is better to formulate the conditions more generally as a so-called set of constraints

$$f_i(\vec{r}) = 0$$

where the index i runs over the number of restrictions, in the above example it would be from one to two. That the right-hand is zero can always be achieved by a subtraction, if need be. To formulate them would not require to fix the geometry of the tube.

A simpler example would be the movement of particle which is required to move on a circle with radius R . In this case, there would be two constraints,

$$\begin{aligned} f_1(\vec{r}) &= z = 0 \\ f_2(\vec{r}) &= \vec{r}^2 - R^2 = 0. \end{aligned}$$

The first constraint requires the particle to move in the plane of the circle. The second constraint then further enforces it to move along the circle. This also shows that the constraints are not unique. E. g., $f_2 = |\vec{r}| - R$ would equally well be possible. The number of independent constraints is, however, unique. In a sense, the constraints reduce the full vector space of coordinates to a subspace, which has a determined number of dimensions.

Such constraints actually eliminate redundant information. In the previous example, the two additional coordinates did not carry any information relevant to the movement of the particle: These information could be completely reconstructed using the one remaining coordinates as well as the constraints. In fact, the constraints could be thought of as

the construction principle for a one-dimensional vector space of non-trivial geometry. It is actually this idea which will be formalized in the following, though this will not be obvious. In fact, the aim will be to make a further step in section 5.13 to transform into a second vector space in which the problem becomes trivial. All non-trivial information will then be contained in the maps between the three vector spaces. The first map will transform from a vector space with constraints to a vector space without constraints and less dimensions, but non-trivial metric. The second map will then transform to a vector space with the same number of dimensions, but with trivial metric.

Before embarking on this process, there are a few more words to be said about the type of constraints.

So far, the constraints only involved a single particle. However, many problems of section 2 did involve multiple particles¹. Correspondingly, if a problem involves several particles the constraints can involve the coordinates of some or all particles,

$$f_j(\vec{r}_1, \dots, \vec{r}_n) = 0$$

if there are n particles. Thus, the dn -dimensional coordinate space, where d is the number of space(-time) dimensions, is reduced to a $dn - N$ dimensional space if there are N constraints. As an example, consider a rigid body made up of M discrete particles with individual masses. This rigidity would then be encoded by $M(M - 1)$ conditions

$$(\vec{r}_i - \vec{r}_j)^2 - c_{ij}^2 = 0,$$

where the matrix c_{ij} is symmetric with $c_{ii} = 0$.

So far, all of the constraints did only involve the coordinates. In general, this is not necessary. Constraints, which are of this form are called holonom-skleronom. Alternatives can be that they include explicitly the time²,

$$f_j(\vec{r}_1, \dots, \vec{r}_n, t) = 0$$

which is then called a holonom-rheonom constraint. E. g., a particle which moves in an elevator, which itself moves along the z -direction with constant speed v would have the constraint

$$z - z_0 - v(t - t_0) = 0. \tag{4.1}$$

¹Continuous mass distributions will usually imply constraints for the center-of-mass, as well as those which guarantee internal rigidity of the body. Fluid dynamics, to be touched upon in section 6.3, is again a different issue.

²In a relativistic treatment time and space are treated equally, and this distinction makes no sense any more. It thus applies only to the non-relativistic case.

This shows that constraints can be as well formulated using only the individual coordinates, rather than with vectors. This can be helpful in practice. However, a formulation involving only vectors is often better to make the symmetries of the problem, if any, more explicit.

If the constraint involve also other quantities, especially speeds or acceleration, they are also no longer holonom. Note that the above example (4.1) could also be formulated as $d_t z - v_0 = 0$, and could therefore also be considered as a non-holonom constraint.

A particular case of non-holonom constraints are those which are inequalities. In such a case the constraints do not reduce the number of degrees of freedom. The following construction can therefore only be applied to a very limited extent.

Note that if there are multiple constraints, they may be of mixed type, e. g. one holonom and one non-holonom constraint. In such cases the following machinery can therefore possibly only be applied partially, and some non-holonom constraints may remain.

Finally, any set of constraints which do not specify a system with only independent coordinates is also not holonom.

4.2 Generalized coordinates

Once the set of constraints are known, it appears reasonable to indeed make the transformation from the ordinary position space to a new space. This space is known as the configuration space. It is a, as noted above, $dn - N$ -dimensional space, the so-called configuration space. The $dn - N$ coordinates of this space are called generalized coordinates. Note that the number of generalized coordinates does not correlate with the number of involved particles, which would be the case for ordinary coordinates.

To qualify as a generalized coordinate two conditions must be met. The first condition is the, somewhat redundant, statement that all coordinates are independent in the sense that no constraints involving them exists. Especially all coordinates can range over the full domain of definition. However, they do not need to be a usual coordinate in the sense that they vary from $-\infty$ to $+\infty$. In the above example of a particle moving on a circle a choice for the generalized coordinate is the angle along the circle, and would thus only vary between 0 and 2π .

The second condition is that there is a unique relation between the generalized coordinates and the original coordinates: It must be possible to reconstruct the position of the particles in position space from the configuration space at every instance of time unambiguously.

This said, the generalized coordinates are not necessarily unique, just their number. E. g. in the case of the circle it would be equally valid to choose the double angle or half

the angle. Furthermore, as this case already indicates, the generalized coordinates are not necessarily coordinates in the usual sense. In case of the angle, a quantity measured in meters has been transformed into an angle. Much more different coordinates will be found later. E. g. a generalized coordinate may equally well be a speed or acceleration, or even the time. As long as it is an unconstrained and unambiguous description of the system, it is useful.

Of course, once such generalized coordinates have been defined, it is possible to derive them with respect to the time, yielding generalized speeds. After a second derivative the generalized accelerations are created.

Since the generalized coordinates uniquely determine all ordinary coordinates, the system is completely described by them. Thus, when rewriting the equations of motions in terms of the generalized coordinates, thereby eliminating a number of them as they are trivially satisfied by the constraints and having only $dn - N$ in the end, the behavior of this system is then fully described by these new equations of motions. These will be in general again second-order differential equations, requiring therefore $2(dn - N)$ initial conditions, e. g. the values of the generalized coordinates and speeds at some time t_0 . Then, the behavior of the system is uniquely characterized by the so-obtained trajectory in the configuration space.

As an example for generalized coordinates take the movement of a particle on the surface of the earth, approximated by a sphere. Then there is one constraint

$$\vec{r}^2 - R^2 = 0$$

and thus there are two generalized coordinates. A useful choice are the angles θ and ϕ which are defined as

$$\begin{aligned}\theta &= \cos^{-1} \frac{z}{R} \\ \phi &= \tan^{-1} \frac{y}{x}\end{aligned}$$

and from which the original coordinates can be reconstructed as

$$\begin{aligned}x &= R \sin \theta \cos \phi \\ y &= R \sin \theta \sin \phi \\ z &= R \cos \theta\end{aligned}$$

This result also emphasizes an important statement. While for every set of values of the generalized coordinates θ and ϕ there is a unique set of ordinary coordinates x , y , and z , the reverse is not true. At the poles the map to the configuration space is not unique. However, the trajectory both in position and configuration space remains unambiguous.

It is an interesting observation that a non-trivial trajectory in configuration space in this case, $(\phi, \theta) = (t, 0)$ translates to a trivial one in position space $(0, 0, R)$, though the translation is unique. This emphasizes that the usual intuition of position space may not be easily translated to configuration space, and vice versa.

Though not at first obvious, the process of introducing generalized coordinates can also be useful even if there are no constraints. This is, e. g., the case if the generalized coordinates are better suited for a particular problem if they are adapted to the symmetry of a problem. E. g. for a potential which is symmetric around the z -axis it is useful to transform from the usual Cartesian coordinates to cylinder coordinates, as they are better suited for this problem. Though this is usually done already in Newtonian mechanics, it is for more involved problems simpler to use the machinery to be developed below.

4.3 The principle of d'Alembert

The aim is now to find the equations of motions for the generalized coordinates without knowing the constraining forces explicitly.

To do, it is useful to introduce the concept of virtual movement. This is best done by first refining the definition of a real movement.

A real movement is what happens to a particle when it moves along its trajectory. If time proceeds by an infinitesimal amount dt , the coordinates r , generalized or otherwise, change by an amount $dr = (dr/dt)dt$. The precise value of dr is determined by the equations of motion.

In contrast, a virtual displacement δr is defined to be an instantaneous change of the coordinates, i. e. $\delta t = 0$. The virtual displacement have to be compatible with the constraints. The symbol δ is used instead of d to distinguish both cases. Such a virtual displacement is also called a variation. Such variations are also taken to be infinitesimal for now, and thus they can be used like ordinary differentials. Especially, these variations are not associated with a speed, and are not constrained by the equations of motion.

Though no power is obtained by such a variation, it is possible to define the work done by a variation for a particle i as

$$\delta W_i = \vec{F} \delta \vec{r}_i.$$

The force \vec{F}_i has two components, $\vec{F} = \vec{K} + \vec{Z}$. The force \vec{Z} is here the constraining force, i. e. the forces which act such that the constraints are fulfilled. The force \vec{K} are all other forces. In the example of the particle in a tube under the influence of gravity in section 4.1, \vec{K} is the gravitational force and \vec{Z} are the forces exerted by the walls of the tube on the particle.

Since Newton's law (2.2), $m d_t^2 \vec{r} = \vec{F}$, still applies

$$\sum_i (\vec{K}_i + \vec{Z} - m_i d_t^2 \vec{r}) \delta \vec{r}_i = 0 \quad (4.2)$$

follows. Now comes the basic step. This has been formulated using Newton's law. Now, this will be turned around, and a new basic postulate will be made. This, and further steps, will replace in the end Newton's laws, and they will ultimately be derived from them backwards. This will take some time.

The first new postulate is then

$$\sum_i \vec{Z}_i \delta \vec{r}_i = 0, \quad (4.3)$$

i. e. constraining forces do no net work. Of course, they can do work on a part of the system, i. e. a subset of the particles. But the total work done by them is zero. Though this postulate cannot be derived, it makes sense in an intuitive ways: If one displaces a particle in a way where it does not violate the constraints, no force has to act, and thus no work to be done, to maintain the constraints.

As an example, consider a particle which moves along some arbitrary curve and which is forced on the curve by constraining forces. Any displacement δr along the curve will then not require any work by the constraining forces. This appears again obvious, as the forces to keep the particle on the curve need to act transversely to the curve only, since any move along the curves coincides with the constraints. Thus, $\vec{Z} \delta \vec{r} = 0$.

An equivalent formulation of (4.3) is obtained by using (4.2),

$$(\vec{K}_i - d_t \vec{p}_i) \delta \vec{r}_i = 0, \quad (4.4)$$

the so-called principle of d'Alembert. This gives another interpretation of the constraining forces: They can be considered as the loss of the forces \vec{K}_i compared to the attained accelerations $d_t \vec{p}_i$. Then the principle of d'Alembert states that these losses do not perform work if a virtual displacement compatible with the constraints is performed. The formulation of d'Alembert embodies already one of the central goals of the current chapter: It no longer references the constraining forces, while it still is an equation of motion which can be solved. In fact, it is already useful for sufficiently simple problems, but it is hard to generalize to more complex one. Therefore, it is only an intermediate stage.

4.4 Euler-Lagrange equations of the second kind

4.4.1 Reformulating d'Alembert's principle

To make progress to a more convenient formulation, it is helpful to recognize the limitations of (4.4): The displacements $\delta\vec{r}_i$ are not independent, but restricted by the constraints. To make it more useful, the next step is to eliminate also the constraints by switching to generalized coordinates.

Since the usual coordinates are differentiable functions of the generalized coordinates, the virtual displacements in terms of the generalized coordinates are given by

$$\delta(\vec{r}_i)_j = \frac{\partial(\vec{r}_i)_j}{\partial q_k} \delta q_k, \quad (4.5)$$

where it was used that, apart from the constraints, virtual displacements are just ordinary differentials, and no time elapses. The index k runs over the number of generalized coordinates. Note that the generalized coordinates can usually not be assembled in vectors like the ordinary coordinates.

This leaves to transfer the momenta in (4.4) to the generalized case. This is somewhat more involved. To simplify matters in the following the mass of the particles will be considered as constant in time. The general case is more involved, but leads ultimately to the same results. As a first step consider

$$\begin{aligned} (d_t \vec{p}_i) \delta \vec{r}_i &= \sum_i m_i (d_t^2 \vec{r}_i) \delta \vec{r}_i \stackrel{(4.5)}{=} \sum_{ij} m_i (d_t^2 \vec{r}_i) \frac{\partial \vec{r}_i}{\partial q_j} \delta q_j \\ &= \sum_{ij} m_i \left(d_t \left(d_t \vec{r}_i \frac{\partial \vec{r}_i}{\partial q_j} \right) - (d_t \vec{r}_i) d_t \frac{\partial \vec{r}_i}{\partial q_j} \right) \delta q_j, \end{aligned} \quad (4.6)$$

where in the last step a zero was introduced.

Now the coordinates can depend both implicitly through the generalized coordinates and explicitly on time, and thus

$$d_t \vec{r}_i = \frac{\partial \vec{r}_i}{\partial q_j} d_t q_j + \frac{\partial \vec{r}_i}{\partial t}.$$

Deriving both sides with respect to $d_t q_j$ yields

$$\frac{\partial d_t \vec{r}_i}{\partial d_t q_j} = \frac{\partial \vec{r}_i}{\partial q_j} \quad (4.7)$$

and thus the total time derivatives drop out. Furthermore

$$d_t \frac{\partial \vec{r}_i}{\partial q_j} = \frac{\partial^2 \vec{r}_i}{\partial q_l \partial q_j} \frac{d q_l}{d t} + \frac{\partial^2 \vec{r}_i}{\partial t \partial q_j} = \frac{\partial}{\partial q_j} \left(\frac{\partial \vec{r}_i}{\partial q_l} d_t q_l + \frac{\vec{r}_i}{\partial t} \right) = \frac{\partial d_t \vec{r}_i}{\partial q_j}. \quad (4.8)$$

Hence, the partial derivative with respect to the generalized coordinates and a total derivative with respect to time commute for the coordinates.

Using both insights in (4.6) yields

$$\begin{aligned} & \sum_{ij} \left(m_i d_t \left((d_t \vec{r}_i) \frac{\partial d_t \vec{r}_i}{\partial d_t q_j} \right) - (d_t \vec{r}_i) \frac{\partial d_t \vec{r}_i}{\partial q_j} \right) \delta q_j \\ &= \sum_{ij} m_i \left(d_t \left(\frac{\partial}{\partial d_t q_j} \left(\frac{1}{2} (d_t \vec{r}_i)^2 \right) \right) - \frac{\partial}{\partial q_j} \left(\frac{1}{2} (d_t \vec{r}_i)^2 \right) \right) \\ &= \left(d_t \frac{\partial T}{\partial d_t q_j} - \frac{\partial T}{\partial q_j} \right) \delta q_j, \end{aligned}$$

and thus the work done by the virtual displacement is given by an expression of derivatives of the kinetic energies with respect to the generalized coordinates and their time derivatives.

Similarly, the first term in (4.4) can be rewritten as

$$\vec{K}_i \delta \vec{r}_i = \vec{K}_i \frac{\partial \vec{r}_i}{\partial q_j} \delta q_j = Q_j \delta q_j,$$

which defines the generalized forces Q_j . Note that just as the generalized coordinates the generalized forces are no vectors, and usually do not even have dimensions of forces. Still, the expression $Q_j \delta q_j$ has the dimension of an energy. But the generalized forces inherit one particular important feature from the forces: If the forces can be obtained from a potential V ,

$$(\vec{K}_i)_j = - \frac{\partial V}{\partial (\vec{r}_i)_j},$$

then the generalized forces are analogously obtained from the same potential when expressed as a function of the generalized coordinates

$$Q_j = - \frac{\partial V}{\partial q_j}, \quad (4.9)$$

recovering the eminent importance of the potential.

This yields d'Alembert's principle (4.4) in terms of the generalized coordinates

$$\left(d_t \frac{\partial T}{\partial d_t q_j} - \frac{\partial T}{\partial q_j} - Q_j \right) \delta q_j = 0 \quad (4.10)$$

which satisfies our wish to also eliminate all explicit appearances of the constraints.

While d'Alembert's principle is very general, as at no time it was used what kind of constraints there are, and in the final expression with the kinetic energy also again time-dependent masses can be used, this form is in many cases far too general. The arguably

most important special case is that of holonom and conservative systems. In fact, all fundamental laws of nature, which have been experimentally confirmed so far, are of this type. However, in more complex systems the effective description as an emergent form may not be of this type.

If the constraints are holonom, all constraints are independent, and especially all δq_j are independent. Then all δq_j are arbitrary, since they are no longer constrained, and can freely vary. But then the only possibility to satisfy (4.10) is if the expression multiplying the δq_j vanish individually, yielding $dn - N$ independent equations

$$d_t \frac{\partial T}{\partial d_t q_j} - \frac{\partial T}{\partial q_j} = Q_j.$$

Since these are as many independent differential equations of second order as there are independent variables, this set of equations describe the system completely. It is therefore equivalent to Newton's equations of motion (2.2). Of course, as Newton's law it requires $2(dn - N)$ independent initial conditions to solve.

An example for such a situation occurs for so-called Rayleigh dissipation. In this case

$$Q_i = -\beta_{ij} d_t q_j,$$

i. e. the dissipation is proportional and inverse to the speed, where the matrix β allows for some curvature of the dissipative forces. A motion without potential but with ordinary dissipation proportional to the speed is an example of Rayleigh dissipation, as there the generalized coordinates are the usual Cartesian ones.

4.4.2 The Euler-Lagrange equations

On the other hand, if the system is conservative then, because of (4.9), the principle of d'Alembert takes the form

$$\left(d_t \frac{\partial}{\partial d_t q_j} (T - V) - \frac{\partial}{\partial q_j} (T - V) \right) \delta q_j = 0,$$

where it has been used that the potential will not depend on the generalized speeds. Otherwise, since the transformation is unambiguous, the potential would depend on the original speeds, and thus the system would not be conservative. The quantity

$$L = T - V$$

is called the Lagrange function. The Lagrange function is the central quantity for brining together special relativity (and possible general relativity) and quantum physics. For

classical, non-relativistic (quantum) mechanics it will only play a role as an intermediate step to Hamiltonian mechanics in chapter 5. Nonetheless, its central importance for any modern formulation of the fundamental laws of nature cannot be overrated, and is therefore stated here without proof.

Using the Lagrange function, d'Alembert's principle for conservative systems takes the form

$$\left(d_t \frac{\partial}{\partial d_t q_j} L - \frac{\partial}{\partial q_j} L \right) \delta q_j = 0, \quad (4.11)$$

and therefore only involves the Lagrange function and the generalized coordinates. It is worthwhile to emphasize that, since the kinetic energy can depend explicitly on the time, so can the Lagrange function, even though the potential energy does not.

If the constraint equations are holonom and the system is conservative, each term in (4.11) is again independent, and thus yields $dn - N$ equations of motion

$$d_t \frac{\partial L}{\partial d_t q_j} - \frac{\partial L}{\partial q_j} = 0, \quad (4.12)$$

the so-called Lagrange equations of the second kind, or sometimes also Euler-Lagrange equations (of motion)³. Again, these equations require $2(dn - N)$ initial conditions to solve.

Lagrange's equation of the second kind is what had been sought for, as they do no longer contain the constraints nor the constraining forces. However, they are not yet the simplest form to solve problems in mechanics and, as noted, not the best choice to generalize to non-relativistic quantum mechanics. Since relativistic quantum physics is for many actual problems, e. g. in solid state physics, serious overkill and far too complicated, it is very useful to find also a better formulation to generalize to non-relativistic quantum mechanics. This is the aim of the remainder of this and of the next chapter, though this may at intermediate steps again only be obvious with hindsight.

It seems at first sight that a similar simplification is not possible in non-conservative systems. However, in some cases it is possible, if the equations of motions are holonom, such that the sum in (4.10) still decouples, and there is a function U such that

$$Q_i = d_t \frac{\partial U}{\partial d_t q_i} - \frac{\partial U}{\partial q_i}.$$

³That no Lagrange equations of the first kind have appeared yet is due to the fact that historically the equations of the first kind had been discovered earlier in a logical progression, while with hindsight it is better to first derive Lagrange's equation of the second kind first and only afterwards in section 4.7 those of the first kind. Still, the historical numbers stuck, as they do so often.

The function⁴ $U(q_i, d_t q_i, t)$ is then called a generalized potential, and the Lagrange function

$$L = T - U \quad (4.13)$$

fulfills formally the same equations (4.12). This seems to be a rather drastic condition for the generalized potential. However, in practice it turns out that there are many systems, most notably when including electromagnetism, which fall into this category. Many of the following calculations hold still true if the generalized potential rather than the normal potential appears.

4.4.3 Examples

It is useful to exhibit the basic strategy with examples.

First consider the so-called fall machine of Atwood. These are two (different) masses m_i exposed to a homogeneous gravitational field of strength g , and which are connected somehow such that given the $z_1 = z$ position of one particle the other can be found at $z_2 = l - z$. This already implements the constraint, yielding only a single relevant coordinate z . The system is conservative, and the constraints are time-independent. The Lagrange function is therefore

$$L = T - V = \frac{1}{2} (m_1 + m_2) (d_t z)^2 - m_1 g z - m_2 g (l - z).$$

The single Euler-Lagrange equation is then

$$d_t \frac{\partial L}{\partial d_t z} - \frac{\partial L}{\partial z} = d_t ((m_1 + m_2) d_t z) - (m_1 - m_2) g = (m_1 + m_2) d_t^2 z - (m_1 - m_2) g = 0$$

The equation of motion is thus

$$d_t^2 z = \frac{m_1 - m_2}{m_1 + m_2} g,$$

I. e., depending on which mass is heavier, the one mass will move up and the other move down with a reduced gravitational acceleration. While the usage of the Lagrange formalism is probably overkill for this problem, it nicely illustrates that the constraints do not appear explicitly in the Lagrange function. Note, however, that in this solution the particles will move to $\pm\infty$, while in truth something will happen when one of the masses reaches the connection point. This is not seen in the solution as this was not encoded in the original description, and especially was not part of the constraints. In the end, also

⁴The notation $f(q_i)$ will here and hereafter signal that the function f depends on all q_i , not only on a single one, to abbreviate the notation. Likewise $f(q_i, d_t q_i)$ depends on all q_i and $d_t q_i$, as well as any kind of generalization to other sets of variables.

the Lagrange formalism can only yield information about a system to the extent it was accurately described.

As a second example, consider a particle moving along a stick which rotates in the plane with a fixed angular velocity ω , but without any external force and thus $V = 0$. This implies two constraints, which can be formulated as, e. g.,

$$\begin{aligned} z &= 0 \\ y - x \tan \omega t &= 0. \end{aligned}$$

Of course, the angular component could have been attached to the coordinate y as well. These constraints are rheonom-holonom, as they explicitly involve the time. A possible generalized coordinate is the distance to the origin where the stick is fixed, $q = r$. The transformations are then given by

$$x = q \cos \omega t \quad (4.14)$$

$$y = q \sin \omega t \quad (4.15)$$

$$z = 0, \quad (4.16)$$

yielding the Lagrange function

$$L = T - V = \frac{m}{2} ((d_t x)^2 + (d_t y)^2) = \frac{m}{2} ((d_t q)^2 + q^2 \omega^2).$$

This yields the Euler-Lagrange equations

$$m d_t^2 q - m \omega^2 q = 0.$$

These equations boil down to the exponential equation

$$d_t^2 = \omega^2 q,$$

and are independent of the mass. Solving yields

$$q(t) = \frac{(d_t q)(0) + \omega q(0)}{2\omega} e^{\omega t} - \frac{(d_t q)(0) - \omega q(0)}{2\omega} e^{-\omega t},$$

which can be inserted into (4.14-4.16) to obtain the final result. The particle moves exponentially outwards, if it is located somewhere on the stick, as long as not $(d_t q)(0) + \omega q(0) = 0$ is satisfied, in which case it is moving to the center. Note that for the choice of suitable initial conditions it is necessary to keep in mind that $q \geq 0$, as it is the positive definite radius. Solving the same problem in Cartesian coordinates would have yielded a product of oscillatory and exponential behavior, which is more involved.

4.4.4 Equivalence to Newton's law

To see that the formulation is equivalent to Newton's law (2.2), consider a conservative system of a single particle without constraints. The general case can also be done, but is somewhat more involved. In this case, there is a potential $V(\vec{r})$. The Euler-Lagrange equations are then

$$L = \frac{m}{2}(d_t\vec{r})^2 - V(\vec{r})$$

$$d_t \frac{\partial L}{\partial d_t r_i} - \frac{\partial L}{\partial r_i} = m d_t(d_t r_i) - \frac{\partial V}{\partial r_i} = m d_t^2 r_i - F_i = 0.$$

The three Euler-Lagrange equations are therefore exactly Newton's second law (2.2) in component form. Since Newton's first and third law are special cases of the second law - the action-reaction relations appear in the n -body version - they are satisfied as well. Only the mathematical framework postulated around Newton's laws in section 2.2 has to be furthermore carried over as well. But since they are related to the arena of mechanics rather than to the dynamics, this was to be expected.

4.5 Invariances of Lagrange's equation of the second kind

Newton's law (2.2) was written in terms of vectors. It therefore had the same form in any coordinate system, and specifying the actual coordinate system is only necessary if it is needed to evaluate it component-wise. Lagrange's equation of the second kind (4.12) are not given as vectorial equations. Since furthermore the choice of generalized coordinates is not unique, it is an important question whether when changing from one set of generalized coordinates to another the equations change form, which would seriously impede their usefulness.

This is not so, as can be seen as follows. Consider an arbitrary, invertible transformation of the generalized coordinates q_i to new coordinates Q_i , i. e.

$$Q_i = Q_i(q_1, \dots, q_s, t)$$

$$q_i = q_i(Q_1, \dots, Q_s, t),$$

with $s = dn - N$ the number of generalized coordinates, which must stay the same. Such a transformation is also called a point transformation, as it assigns to any point in the new coordinates exactly one point in the old coordinates. For simplicity again only conservative

systems with holonom constraints will be considered. In the same way as for (4.7-4.8) it can be shown that

$$\begin{aligned}\frac{\partial d_t q_i}{\partial d_t Q_k} &= \frac{\partial q_i}{\partial Q_k} \\ d_t \frac{\partial q_i}{\partial Q_k} &= \frac{\partial d_t q_i}{\partial Q_k},\end{aligned}$$

which will be needed in the following. Furthermore, it is necessary to note that the Lagrange functions in the new coordinates is obtained by writing

$$L(Q_1, \dots, Q_s, t) = L(Q_1(q_1, \dots, q_s, t), \dots, Q_s(q_1, \dots, q_s, t), t) = L(q_1, \dots, q_s, t)$$

and can therefore be considered as function of both the new and the old coordinates. However, its actual functional form may be different, as will be seen in actual calculations.

To piece together (4.12) in the new coordinates requires three ingredients

$$\begin{aligned}\frac{\partial L}{\partial Q_i} &= \frac{\partial L}{\partial q_j} \frac{\partial q_j}{\partial Q_i} + \frac{\partial L}{\partial d_t q_j} \frac{\partial d_t q_j}{\partial Q_i} \\ \frac{\partial L}{\partial d_t Q_i} &= \frac{\partial L}{\partial d_t q_j} \frac{\partial q_j}{\partial Q_i} \\ d_t \frac{\partial L}{\partial d_t Q_i} &= \left(d_t \frac{\partial L}{\partial d_t q_j} \right) \frac{\partial q_j}{\partial Q_i} + \frac{\partial L}{\partial d_t q_j} \frac{\partial d_t q_j}{\partial Q_i}.\end{aligned}$$

Subtracting the first from the third line yields

$$d_t \frac{\partial L}{\partial d_t Q_i} - \frac{\partial L}{\partial Q_i} = \left(\left(d_t \frac{\partial L}{\partial d_t q_j} \right) - \frac{\partial L}{\partial q_j} \right) \frac{\partial q_j}{\partial Q_i} = 0,$$

where it has been used that the Euler-Lagrange equations hold in the variables q_i , and therefore the parentheses vanishes for every value of j separately. Thus, the Euler-Lagrange equations are indeed form invariant under any transformation of the generalized coordinates.

There is another invariance of the Euler-Lagrange equations, which is very useful. Choose some Lagrange function and an arbitrary (twice differentiable) function $f(q_i, t)$ depending only on the generalized coordinates and the time. Then the Lagrange function

$$L^f = L + d_t f = L + \partial_t f + \frac{\partial f}{\partial q_i} d_t q_i, \quad (4.17)$$

has the same Euler-Lagrange equations. This can be seen by considering the Euler-Lagrange equations for the additional term,

$$\begin{aligned}\frac{\partial d_t f}{\partial q_i} &= \frac{\partial^2 f}{\partial t \partial q_i} + \frac{\partial^2 f}{\partial q_i \partial q_j} d_t q_j \\ d_t \frac{\partial d_t f}{\partial d_t q_i} &= d_t \frac{\partial}{\partial d_t q_i} \left(\partial_t f + \frac{\partial f}{\partial q_i} d_t q_i \right) = d_t \frac{\partial f}{\partial q_i} = \frac{\partial^2 f}{\partial t \partial q_i} + \frac{\partial^2 f}{\partial q_i \partial q_j} d_t q_j,\end{aligned}$$

which are therefore identically zero. Note that it was important that the function f is continuously differentiable, because swapping the derivatives would otherwise not be possible. It was also important that the total time-derivative was added to the Lagrangian, as the cancellation would have not worked if it would have been only a partial one. This is significant, as will be seen later in section 5.1. Such an addition of a total time derivative is sometimes called a (mechanical) gauge transformation, but this terminology will not be used here, as the more general idea of gauge theories will supersede it in classical field theory and quantum field theory.

4.6 Generalized momenta and cyclic coordinates

To continue, it is helpful to introduce a new concept, the so-called generalized momenta. They are defined as

$$p_i = \frac{\partial L}{\partial d_t q_i}. \quad (4.18)$$

Even for a particle, the generalized momenta will in general not coincide with $md_t q_i$, though they may.

If the Lagrange function does not depend on a given coordinate

$$\frac{\partial L}{\partial q_i} = 0$$

it follows that

$$0 = d_t \frac{\partial L}{\partial d_t q_i} - \frac{\partial L}{\partial q_i} = d_t p_i.$$

Thus, the p_i must be constant. Thus the quantity p_i is conserved. As has been seen in section 2.7 such conserved quantities, sometimes also called integrals of motion, are very useful, as the corresponding motions are trivial. Is this the case the corresponding coordinate q_i is called cyclic.

Finding thus generalized coordinates in which as many as possible coordinates are cyclic makes problems therefore much simpler to solve. How to do so systematically will be discussed further in section 5.13, after further tools have been introduced to achieve this goal.

An interesting example for this is obtained for the case of a single free particle. Its Lagrange function reads

$$L = \frac{m}{2} (d_t \vec{x})^2.$$

In this case the coordinates are all cyclic, implying the existence of 3 conserved quantities, the corresponding generalized momenta. These are

$$p_i = \frac{\partial L}{\partial d_t x_i} = m_i d_t x_i$$

which therefore coincide with the usual momenta. Using the conventional approach, this would have required to solve already the equations of motion. In fact, the Euler-Lagrange equations are

$$d_t \frac{\partial L}{\partial d_t x_i} = m_i d_t^2 x_i = 0$$

and therefore coincide once more with Newton's law (2.2).

A less trivial example is the Kepler problem of section 2.7.3. In this case, suitable generalized coordinates are spherical coordinates

$$x = r \cos \phi \sin \theta \quad (4.19)$$

$$y = r \sin \phi \sin \theta \quad (4.20)$$

$$z = r \cos \theta \quad (4.21)$$

as it is a central potential. The corresponding Lagrange function is

$$L = \frac{m}{2} ((d_t r)^2 + r^2 (d_t \theta)^2 + r^2 (d_t \phi)^2 \sin^2 \theta) + \frac{\alpha}{r},$$

where m is the reduced mass, α is the strength of the gravitational interaction, usually $G_N m_1 m_2$, r is the radial distance between both bodies, and θ and ϕ are the azimuth angle and polar angle, respectively. There is one cyclic coordinate with the conserved generalized momentum

$$p_\phi = m r^2 (d_t \phi) \sin^2 \theta = l_z$$

which is identified as the z -component of the angular momentum. Thus, the movement in a plane is yielded by the Lagrange formalism much easier than before. Note that this result holds true for any ϕ -independent potential. Solving the remaining equations of motion is in this particular problem not substantially easier than before. The reason is, however, that in section 2.7.3 already the generalized coordinates had been used. Would the Cartesian coordinates have been used, the situation would be much different.

4.7 Lagrange's equation of the first kind

If the constraints are non-holonom, it is not possible to go beyond (4.10) in the previously formulated way. In some of these cases Lagrange's equations of the first kind can be useful. Furthermore, during developing them a powerful technique, that of Lagrange multipliers, will be introduced which is very useful to implement constraints in much more general settings, ranging from thermodynamics and statistical physics to solving numerical problems. In general, their purpose is also to implement constraints, but not necessarily for mechanical systems only.

The method of Lagrange multipliers is particularly suited if the constraints themselves contain derivatives and cannot be integrated. Consider for the following a system where M of the N constraints are non-holonom. A useful way to write the constraints of this type is

$$f_{ji}(q_1, \dots, q_r, t) dq_i + f_j(q_1, \dots, q_r, t) dt = 0, \quad (4.22)$$

where j runs from 0 to M . The constraints are hence formulated as differentials and the holonom constraints have already been used to transform to generalized coordinates as far as possible. Thus, $r = dn - N + M$ and $i = 1, \dots, r$.

Now, under any kind of virtual displacement $dt = 0$, and the remaining constraints have the form

$$f_{ji} \delta q_i = 0. \quad (4.23)$$

If this is true, then also any sum of these statements is true. Therefore multiply all M equations by an arbitrary functions of time, but not of the coordinates, and add them. This yields

$$\lambda_j(t) f_{ji} \delta q_i = 0$$

where the (so far) arbitrary M functions λ_i are called Lagrange multiplier for reasons to be seen. They are also called constants, despite their time-dependence, as they do not depend on the coordinates.

If the system is conservative, or there is at least a generalized potential, the condition (4.11) still holds. Furthermore, it is possible to add zero to (4.11), and therefore

$$\left(d_t \frac{\partial L}{\partial d_t q_i} - \frac{\partial L}{\partial q_i} - \lambda_j f_{ji} \right) \delta q_i = 0.$$

Since the generalized coordinates are not independent, the separate terms in parentheses are not zero individually.

However, though it was not possible to resolve the generalized constraints, they are still constraints. Thus, out of the r generalized coordinates only $dn - N = s$ are independent. Since the choice of which are dependent and which are independent is arbitrary, it is useful to order them, and choose the first $i = 1, \dots, s$ to be independent and the remaining ones $i = s + 1, \dots, r$ to be dependent on the former.

Now assume that there exist values for the λ_j such that

$$d_t \frac{\partial L}{\partial d_t q_i} - \frac{\partial L}{\partial q_i} - \lambda_j f_{ji} = 0$$

for $i = s + 1, \dots, r$, i. e. M equations for the dependent variables. It appears at first sight highly non-trivial that some, in general time-dependent, quantities λ_j should exist

such that this relation between functions should be correct. However, the two parts of the equations actual express the same statement, i. e. the fact that these $q_{s+1\dots r}$ are not independent variables, once formulated using the Lagrange function and once formulated using the constraints. They thus contain the same information, only in different ways. By superimposing all possibly ways how to express the dependence of the generalized coordinates by summing over all constraints, it is taken care of that the Lagrange function expresses the same information in a different way. Thus it appears reasonable that such values for the λ_j exist, and indeed this is the case. The same could be achieved by rather multiplying the terms involving the Lagrange function and summing them and adding single constraints, as this is exactly the same information content. However, for practical use this form is more adequate.

But since the remaining generalized coordinates $q_{i\dots s}$ are independent, so are their virtual translations δq_i , and hence

$$d_t \frac{\partial L}{\partial d_t q_i} - \frac{\partial L}{\partial q_i} - \lambda_j f_{ji} = 0 \quad (4.24)$$

for $i = 1, \dots, s$ as well. These are Lagrange's equation of the first kind. However, they are not alone sufficient. The constraints (4.22) have not been resolved, and still needed to be solved simultaneously. Thus, it is necessary to solve $N + M$, rather than N equations for the $q_{1\dots N}$ functions as well as for the M parameters λ_j .

Though these are now more equations to solve, the advantage is that more information is gained as well. Since the constraints are related to the constraining forces, some knowledge about them is gained. This becomes visible when comparing (4.24) with (4.10). The expressions

$$\tilde{Q}_i = \lambda_j f_{ji},$$

act like generalized forces, and can therefore be considered to be a generalized constraining force. In fact, if knowledge about the constraining forces in the case of holonom constraints is required, Lagrange's equations of the first kind can be used as well. A holonom constraint F can be transformed into a non-holonom one by considering

$$dF = \frac{\partial F}{\partial q_i} dq_i + \frac{\partial F}{\partial t} dt = 0,$$

and the derivatives of the constraint therefore take the role of the f_{ji} and f_j in (4.22).

It is useful to consider an example. Take a hollow cylinder rolling down a hill. Its moment of inertia is $J = mR^2$, where R is its radius. Since it can only move along the hill, the generalized coordinates can be chosen to be the the distance along the hill $q_1 = x$. To actually apply Lagrange's equation of the first kind requires a dependent

further generalized coordinate. This will be the angle of rotation of the cylinder, $q_2 = \theta$. The cylinder should stay rigid and therefore the constraint is

$$Rd\theta - dx = Rdq_2 - dq_1 = 0.$$

The one non-holonom constraint has therefore $f_{11} = -1$, $f_{12} = R$, and $f_1 = 0$. Assume that gravity is acting on the cylinder, making it roll. The Lagrange function of this (conservative) system is then given by

$$L = \frac{m}{2}(d_t q_1)^2 + \frac{J}{2}(d_t q_2)^2 - mgq_1 \sin \phi,$$

where ϕ is the inclination of the hill.

There is only one Lagrange parameter, λ_1 . The two equations of the first kind of Lagrange and the one obtained from the constraints read

$$\begin{aligned} d_t \frac{\partial L}{\partial q_1} - \frac{\partial L}{\partial q_1} - \lambda_1 f_{11} &= md_t^2 q_1 - mg \sin \phi + \lambda_1 = 0 \\ d_t \frac{\partial L}{\partial q_2} - \frac{\partial L}{\partial q_2} - \lambda_1 f_{12} &= Jd_t^2 q_2 - R\lambda_1 \\ -d_t q_1 + Rd_t q_2 &= 0. \end{aligned}$$

It is important to note here that, even though q_2 is cyclic, this does not yield a conservation law in this case, because this applied for independent coordinates.

Deriving the constraint equation once more yields

$$-d_t^2 q_1 + Rd_t^2 q_2 = 0,$$

and thus a relation between the second-order derivatives of the generalized coordinates. Then three times the same unknowns appear linearly in the equations, and it is possible to decouple them, yielding

$$\begin{aligned} d_t^2 q_1 &= \frac{g \sin \phi}{2} \\ d_t^2 q_2 &= \frac{g \sin \phi}{2R} \\ \lambda_1 &= \frac{M}{2} g \sin \phi. \end{aligned}$$

The two generalized coordinates are therefore just uniformly accelerated motions, and the Lagrange parameter is in this case a constant. More interesting are the two generalized forces

$$\begin{aligned} \tilde{Q}_1 &= \lambda_1 f_{11} = -\frac{mg \sin \phi}{2} \\ \tilde{Q}_2 &= \lambda_1 f_{12} = \frac{mgR \sin \phi}{2}. \end{aligned}$$

The first is a force opposing the movement of the cylinder, reducing its acceleration compared to the free-fall acceleration of g . The second is the angular acceleration, which makes the cylinder roll. Both are exerted by the forces between the hill and the cylinder, which are actually microscopic electromagnetic forces.

4.8 Conservation laws

In section 4.6 conserved quantities, so-called integrals of motions, have been obtained from cyclic coordinates. While cyclic coordinates always yield a conserved quantity, the converse is not true, and there may be (many) more conserved quantities than there are cyclic coordinates in the Lagrange function. This already follows from the fact that generalized coordinates are not unique, and a coordinate may be cyclic for one choice, but not for another.

This can be seen in the following example. Consider two bodies of different masses which interact via a potential $V(|\vec{r}_1 - \vec{r}_2|)$, but there are otherwise no constraints. In Cartesian coordinates their Lagrange function reads

$$L = \frac{m_1}{2}(d_t \vec{r}_1)^2 + \frac{m}{2}(d_t \vec{r}_2)^2 + V(|\vec{r}_1 - \vec{r}_2|).$$

None of the coordinate is cyclic. But the considerations in section 2.8 have shown that the movement of the center of mass and the relative movements of the particles decouple using center-of-mass coordinates. Introducing these coordinates as generalized coordinates, using the notations of section 2.8.1,

$$\begin{aligned} q_{1\dots 3} &= \vec{R}_{1\dots 3} \\ q_4 &= |\vec{r}_1 - \vec{r}_2| \\ q_5 &= \theta \\ q_6 &= \phi, \end{aligned}$$

where θ and ϕ are the angles in spherical coordinates of $\vec{r} = \vec{r}_1 - \vec{r}_2 = r(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)^T$.

Though tedious, straightforward evaluation yields the Lagrange function in these coordinates

$$L = \frac{M}{2} ((d_t q_1)^2 + (d_t q_2)^2 + (d_t q_3)^2) + \frac{\mu}{2} ((d_t q_4)^2 + q_4^2 (d_t q_5)^2 + q_4^2 (d_t q_6)^2 \sin^2 q_5) + V(q_4),$$

in which four coordinates are cyclic, $q_{1\dots 3}$ and q_6 . Thus, there are immediately four conserved quantities, simplifying the problem tremendously. These are exactly the ones already known, the three components of the momentum of the center of mass, while the fourth is the angular momentum along the z -axis with respect to the center of mass.

Thus, a good choice of generalized coordinates can simplify the problem tremendously. However, finding them is not always simple. Here, some general rules will be described which allow to construct many conserved quantities, while a much more sophisticated approach will be discussed in section 5.13.

4.8.1 Energy conservation

Assume that the Lagrange function does not depend explicitly on the time. Then

$$d_t L = \left(\frac{\partial L}{\partial q_i} d_t q_i + \frac{\partial L}{\partial d_t q_i} d_t^2 q_i \right) = \left(\left(d_t \frac{\partial L}{\partial d_t q_i} d_t q_i \right) + \frac{\partial L}{\partial d_t q_i} d_t^2 q_i \right) = d_t \left(\frac{\partial L}{\partial d_t q_i} d_t q_i \right),$$

where in the second step Lagrange equation's of the second kind have been used, assuming holonom constraints.

Using the generalized momentum (4.18) the Hamilton function is defined as

$$H = p_i d_t q_i - L, \quad (4.25)$$

and which is therefore conserved in time when the Lagrange function does not explicitly depend on time. This function will reappear also in chapter 5.

At first sight, this is a rather abstract conserved quantity. However, for skleronom constraints in a conservative system and if the generalized kinetic energy has the property⁵

$$T(ad_t q_i) = a^2 T(d_t q_i)$$

it is possible to give H a very particular meaning.

In this case

$$d_a T = \frac{\partial T}{\partial(ad_t q_i)} \frac{\partial ad_t q_i}{\partial a} = \frac{\partial T}{\partial(ad_t q_i)} d_t q_i = 2aT,$$

which is true for any a , and therefore also for $a = 1$. This implies

$$H = \frac{\partial L}{\partial d_t q_i} d_t q_i - T + V = 2T - T + V = T + V,$$

and therefore in this case the Hamilton function is just the total energy. Note that for rheonom constraints this is not true, as the constraining forces can then also contribute energy.

Thus, for skleronom and conservative systems, which are by far the most numerous ones and the only ones relevant in fundamental physics, the total energy is conserved if

⁵A function obeying $f(ax) = a^n f(x)$ is said to be homogeneous of order n . The required property of the kinetic energy is therefore homogeneity of order 2.

the Lagrange function does not depend explicitly on time. The absence of explicit time-dependence can also be interpreted in a different way. Any transformation $t \rightarrow t + \Delta t$ will leave in this case both the Lagrange function and the Euler-Lagrange equations unchanged. Thus, the system is homogeneous (or isotropic) in time, as defining any time as $t = 0$ for the initial conditions is equally good, and there is no distinct time. This also explains that fundamental physics is usually of this type: To the best of our knowledge time has no absolute frame, just as discussed in chapter 3.

4.8.2 Momentum conservation

As may be expected from chapter 3, a very similar argument as in the previous section also holds if the space is homogeneous. Homogeneity in space means that everything depends only on relative distances. An example is the central force problem of section 2.7.3: The potential depended only on the relative distance of two particles, $\vec{r}_1 - \vec{r}_2$, rather on their absolute positions. Therefore any shift of the coordinate system $\vec{r}_i \rightarrow \vec{r}_i + \Delta\vec{r}$ would not have changed anything.

Corresponding generalized coordinates would therefore be relative coordinates, just as at the beginning of this section. They are not affected by such changes. The center-of-mass coordinate, which is affected, would therefore be cyclic, just as with the time discussed in case of the homogeneity of time. Thus the corresponding generalized momenta, which is just the center-of-mass momentum, will be conserved.

This is therefore a particular case of section 4.6. The same statement could therefore be read that if a system is translationally invariant, i. e. the absolute position does not matter, in a generalized coordinate, its associated generalized momentum is conserved.

To better understand this generalization, it is best to consider a conservative system. Then for a cyclic coordinate

$$p_i = \frac{\partial L}{\partial d_t q_i} = \frac{\partial T}{\partial d_t q_i} = \sum_j m_j (d_t \vec{r}_j) \frac{\partial d_t \vec{r}_j}{\partial d_t q_i} = \sum_j m_j (d_t \vec{r}_j) \frac{\partial \vec{r}_j}{\partial q_i}, \quad (4.26)$$

where (4.7) has been used. Since by assumption, the system must be invariant under translations in the cyclic coordinates, all coordinates must change in the same way under a change in q_i ,

$$\Delta \vec{r}_i \rightarrow \Delta \vec{r}_i + \Delta q_i \vec{n}_i,$$

and thus the derivative is a unit vector \vec{n}_i in the homogeneous direction,

$$p_i = \sum_j m_j (d_t \vec{r}_j) \vec{n}_i = \vec{n}_i \vec{P},$$

where \vec{P} is the ordinary momentum of the center of mass. Thus, the corresponding component of the center-of-mass momentum is conserved. If space is homogeneous in all directions, this results in three cyclic coordinates, and thus the center-of-mass momentum is fully conserved. The example at the beginning of this section exemplifies this.

The cyclicity implies that the corresponding generalized force vanishes and thus

$$0 = -\frac{\partial V}{\partial q_i} = Q_i = \vec{F}_j \frac{\partial \vec{r}_j}{\partial q_i} = \vec{n}_i \sum_j \vec{F}_j$$

Hence, the projection of the total force in the corresponding direction vanishes.

4.8.3 Angular momentum conservation

A system is called isotropic in space if it does not change under a rotation. Therefore, the corresponding angular variable will again be cyclic, as the system does not depend on it. This has also been exemplified in the example at the beginning of the section. In this case the derivative in (4.26) will not be along a direction \vec{n}_i , but rather be like a rotation of the coordinates,

$$\Delta \vec{r}_i = \Delta q_i \vec{n}_i \times \vec{r}_i.$$

Deriving this relation with respect to q_i then yields

$$p_i = \sum_j m_j (d_t \vec{r}_j) (\vec{n}_i \times \vec{r}_j) = \vec{n}_i \sum_j m_j (d_t \vec{r}_j) \times \vec{r}_j = n_i \vec{L},$$

where \vec{L} is the total angular momentum. Thus, the angular momentum along the rotation axis is conserved. If the system is isotropic for all possible rotation axes, the total angular momentum is conserved.

Given the example in the beginning of this section, the question may at first arise whether it is isotropic, as only the component \vec{L}_z has appeared as a conserved generalized momentum. This is however misleading. In fact, the choice of coordinate system guarantees in the example that the total angular momentum is oriented along the z -axis. Therefore, the two other components vanish by construction, and actually the total angular momentum is conserved. Here it surfaces that the angular momentum is defined by a coordinate system acting as a reference point.

As before, the vanishing of the corresponding generalized force implies that the component of the total torque along the rotation axis vanishes.

4.8.4 Noether's theorem

The previous observations can be generalized in the form of Noether's theorem. It is one of the central reasons why symmetries are so important in physics. It shows that for a holonom and conservative system any continuous symmetry, i. e. a symmetry where a generalized coordinate is change by a continuous quantity, entails the existence of a conservation law. The previous cases were special examples of this, as they amounted to a continuous shift in time, space, and rotation.

Such conserved quantities are of central importance for both theoretical and practical reasons. Practical, because exploiting conservation laws is very helpful in solving problems. Theoretical, conserved quantities define the properties of a system.

Essentially, Noether's theorem boils down to the fact that if the Lagrange function is invariant under a variation of a generalized coordinate, the variation can be used to derive a conserved quantity. To keep it simple, start with a Lagrange function of a single generalized coordinate, $L(q, d_t q)$. The Lagrange function shall now be invariant under the transformation

$$q \rightarrow q + \Delta q,$$

where Δq is taken to be infinitesimal, i. e.

$$L(q + \Delta q, d_t q + d_t \Delta q) = L(q, d_t q).$$

Expanding the left-hand side to first order in a Taylor series yields

$$L(q, d_t q) + \frac{\partial L}{\partial q} \Delta q + \frac{\partial L}{\partial d_t q} (d_t \Delta q) = L(q, d_t q).$$

But this implies

$$0 = \frac{\partial L}{\partial q} \Delta q + d_t \left(\frac{\partial L}{\partial d_t q} \Delta q \right) - d_t \left(\frac{\partial L}{\partial d_t q} \right) \Delta q = d_t \left(\frac{\partial L}{\partial d_t q} \Delta q \right),$$

where in the last step the Euler-Lagrange equations have been used. This must be true for any variations of q , and thus especially for time-independent ones, yielding

$$d_t \frac{\partial L}{\partial d_t q} = 0$$

Thus, the invariance implies a conservation law, and that the corresponding generalized momentum is conserved. Of course, if the coordinate q is cyclic, this just reproduces what was known before. But in general, this implies

$$q'_i = q_i + \Delta q_i$$

$$d_t \left(\frac{\partial L}{\partial d_t q_i} \Delta q_i \right) = 0.$$

This does not look very helpful yet. But rewrite $\Delta q_i = \epsilon f_i$, where the f_i are some arbitrary functions, and ϵ is infinitesimal. Then this is equivalent to

$$d_t \left(\frac{\partial L}{\partial \dot{q}_i} \frac{\partial q'_i}{\partial \epsilon} \right) = 0,$$

i. e., it involves now how a generalized coordinate reacts to a change. These expressions may now be more complicated than just cyclic coordinates.

In this way, conserved quantities are linked to invariances of a system. Such an invariance is also called a symmetry, as the system looks the same, whether using the coordinate q or q' . This is a very fundamental insight that symmetries are connected to conservation laws, and will be encountered throughout all of physics.

4.8.5 Virial's theorem

The conservation laws treated so far hold locally in time, i. e. they are fulfilled at every time t . Though these are very powerful statements, it is also often possible to make weaker, but nonetheless very helpful statements. Such statements are usually describing some average properties of a system. This will become very important when deriving thermodynamics as a limit of the mechanics of many particles, so-called statistical mechanics. Here, as a first example of such statements Virial's theorem will be discussed.

Consider for a system of particles with ordinary coordinates the quantity

$$G = \vec{p}_i \vec{r}_i.$$

Using Newton's law (2.2), its total derivative is given by

$$d_t G = (d_t \vec{r}_i) \vec{p}_i + \vec{r}_i (d_t \vec{p}_i) = m(d_t \vec{r}_i)^2 + \vec{r}_i \vec{F}_i = 2T + \vec{r}_i \vec{F}_i,$$

where T is the kinetic energy.

As announced, the aim is to make a statement about quantities on the average. In Virial's theorem, this will be an average over a time τ . This average is obtained by integrating the time derivative of G over time,

$$\frac{1}{\tau} (G(\tau + t) - G(t)) = \frac{1}{\tau} \int_t^{t+\tau} \frac{dG}{dt} dt = \frac{1}{\tau} \int_t^{t+\tau} (2T + \vec{r}_i \vec{F}_i) dt.$$

If the system is finite in the sense that all positions and momenta stay finite, then G is bounded from above. Thus, by making τ large, the left-hand side can be made arbitrarily

small. For a periodic system, by choosing τ to be the period, it can even be made zero. This yields Virial's theorem

$$\int_t^{t+\tau} T dt = -\frac{1}{2} \int_t^{t+\tau} \vec{r}_i \vec{F}_i dt,$$

where the right-hand side is known as the virial of Clausius. This statement is the starting point for many derivations in the aforementioned statistical mechanics access to thermodynamics.

For many cases also the following particular case of a conservative central potential is interesting, as investigated in section 2.7. Then

$$\vec{r}_i \vec{F}_i = r \partial_r V_i(r),$$

where r is now the distance to the center of the potential. If $V(r)$ is, as often, proportional to some power r^n , then

$$r \partial_r V_i(r) = n V(r),$$

and Virial's theorem takes the form

$$\int_t^{t+\tau} T dt = -\frac{n}{2} \int_t^{t+\tau} V dt$$

and thus the temporal average of the potential energy has a fixed relation to the temporal average of the kinetic energy. While an explicit evaluation of either side still requires to know $\vec{r}(t)$ already knowledge of this relation often is sufficient to answer relevant questions about a system for which the actual trajectories are not important to know.

Chapter 5

Hamiltonian mechanics

So far, the formulation of mechanics has been by use of differential equations, especially Lagrange's equation of the first kind and second kind, (4.24) and (4.12), respectively. Though this approach is extremely useful in mechanics, and also of great practical importance, it is not yet the best formulation to extend it to (non-relativistic) quantum physics. The main reason for this is that quantum physics, especially in combination with special relativity, introduces correlations which are not local, i. e. not describable by differential equations, but also requires non-local aspects, i. e. integrals. Though for classical mechanics both a differential and an integral formulation yield the same result, it is helpful to perform the corresponding conceptual formation already in the otherwise much simpler classical mechanics. It will also help eventually to demonstrate that for many cases it is always possible to find generalized coordinates such that the system becomes that of almost trivial mechanical systems in section 5.13.

Unless otherwise noticed, most of the following will apply to the most relevant case of conservative systems with holonom constraints.

5.1 Hamilton's principle

5.1.1 Integral formulation

The basic entities to formulate the following are constructed from the configuration space, i. e. the $dn - N$ -dimensional space of the independent, generalized coordinates. Any curve inside this space parametrized by a parameter t , no matter whether it is a solution to the equation of motion, is a trajectory describing the movement of the particles of the system.

Consider the solutions of the equations of motion, which are solutions to differential

equations which are of second order in time¹, and therefore require $(2dn - N)$ initial conditions. Though in practice it may be awkward, it is always possible to select two times t_1 and t_2 and specify the initial conditions by the values of all generalized coordinates at those two times, $q_i(t_1)$ and $q_i(t_2)$.

Then it is possible to select among all possible trajectories in the configuration space those which are (twice) differentiable in time and satisfy the initial conditions of the problem at hand. In addition, it will be required that these trajectories must be reachable from a trajectory fulfilling the equations of motions, the so-called physical trajectories, by successive virtual displacements, i. e. the trajectories are dense around the physical trajectories inside the configuration space. However, once this definition is made, any other trajectories inside the set can equally well be used to define it².

This subset of configurations will be called \mathcal{M} . All such trajectories share a number of characteristics, by construction. First of all, they spend trivially the same time between start and end points at t_1 and t_2 . Secondly, all virtual displacements at the initial and final time have to vanish, i. e. $\delta q_i(t_1) = \delta q_i(t_2) = 0$, as otherwise the constraints (in form of the initial conditions) would be violated.

It is now possible to evaluate the Lagrange function on any element of $q(t) \in \mathcal{M}$, yielding a function only of time

$$L(q_i(t), d_t q_i(t), t) = L(t),$$

and it is formally possible to integrate this function over time to yield a number

$$S[q] = \int_{t_1}^{t_2} dt L(t), \quad (5.1)$$

which is called the action. This number depends on the choice $q(t)$, i. e. which trajectory is chosen. It therefore maps a function, or more precisely functions, to the real numbers. This is different from functions, which map values of variables to the real numbers. Such an object has therefore a different name, and is called a functional.

¹Note that this may appear different when, e. g., a speed becomes a generalized coordinates, but this is deceiving. At any rate, there can be no more independent initial conditions than those for all independent coordinates in the formulation using Newton's law (2.2).

²The reason for talking about physical trajectories instead of a single trajectory is to include also cases in which there are two equivalent trajectories, e. g. for moving in both possible directions from one point of the circle to the opposite point. These trajectories are not deformable into each other. Such a situation occurs if there are, like with the circle, holes in a generalized sense. This unusual, but by no means irrelevant, situation will be noted if occurring. Otherwise in the following only a single physical trajectory will be relevant.

After these preparations, it is possible to postulate the principle of Hamilton. There are actually two different ways to postulate it. Again, it will be shown later that this yields the same results as the Euler-Lagrange equations in classical mechanics.

The first version is that the physical trajectory is the one trajectory in \mathcal{M} , which extremalizes the action. It seems to be odd to define the solution using a manifold which was defined using the solution. However, it will turn out that it is in general much simpler to specify \mathcal{M} even without knowing the actual physical trajectory than to solve the system. This postulate already emphasizes the non-local nature of Hamilton's principle. To know the solution requires not only to know the possible trajectories at all times, but the whole set \mathcal{M} . This is very different from the Euler-Lagrange equations or Newton's law, which only needed to know about the function and its derivatives at one point to build the solution. That this is still the more powerful formulation is hence far from obvious.

One advantage is, however, visible: The action does not depend on the coordinate system in configuration space, since it is entirely formulated on paths. It is therefore a coordinate-independent classical mechanics, therefore eliminating the human-made coordinate systems.

5.1.2 Variational formulation

The alternative formulation uses again the concept of virtual displacements. It requires that the physical path is the one where the change of S under virtual displacements of the path in configuration space, $q \rightarrow q + \delta q$, vanishes, expressed as

$$\delta S = 0.$$

While this seems to be a very compact notation, it is mathematically far from obvious what it means: How is the variation of a functional calculated? Understanding this is the first part of functional calculus, which is a wide field, which plays an important role in classical as well as quantum field theory. Here, only those parts will be discussed which will be needed to calculate δS .

Of course, it is not yet obvious that this formulation is equivalent to the integral version, but also this will now be seen. This will amount to the statement that an extremal trajectory has zero variation of the action, which is, not accidentally, reminiscent of the way how extrema of functions are found.

To introduce the concepts, it is best to consider a simplified case, a functional F depending only on a single function f depending in turn on a variable y , which itself depends on a single parameter x . Furthermore, it will be required that the values of y at

the two points x_1 and x_2 are the same for all functions y . The functional F is then defined as

$$F[y(x)] = \int_{x_1}^{x_2} dx f(y, d_x y, x).$$

Note that this is a very special class of functionals, a so-called linear functional. It would be equally well possible to have other forms of the functionals, but these will be of no interest in this lecture.

It will be necessary that both y and f are continuously differentiable functions³.

As the question has already been formulate in this way, the task is now to find a criterion for the extremalization of F as a functional of y . To create a formally well-defined way, split the function y in two parts,

$$y(x) = y_s(x) + \alpha\eta(x),$$

where y_s is the (yet unknown) solution searched for, α is a new, continuous parameter, η is an arbitrary, sufficiently often differentiable function with $\eta(x_1) = \eta(x_2) = 0$. Thus, this is a completely equivalent way of rewriting the class of functions y .

Any infinitesimal change⁴ of the curve y around the solution curve y_s can therefore be replicated by taking α infinitesimal small, denoted as $\delta\alpha$, and some suitable choice of η ,

$$\delta y = y - y_s = \eta \delta\alpha = \left. \frac{dy}{d\alpha} \right|_{\alpha=0} \delta\alpha.$$

The corresponding variation of the functional is then defined as

$$\delta F = F(y) - F(y_s) = \int_{x_1}^{x_2} dx (f(y, d_x y, x) - f(y_s, d_x y_s, x)). \quad (5.2)$$

Since it is assumed that $\delta\alpha$ is infinitesimal, it is possible to expand f in a Taylor series to first order in $\delta\alpha$

$$\begin{aligned} f(y, d_x y, x) &\approx f(y_s, d_x y_s, x) + \delta\alpha d_\alpha f = f(y_s, d_x y_s, x) + \delta\alpha \left(\frac{\partial f}{\partial y} \frac{\partial y}{\partial \alpha} + \frac{\partial f}{\partial d_x y} \frac{\partial d_x y}{\partial \alpha} \right) \\ &= f(y_s, d_x y_s, x) + \delta\alpha \left(\frac{\partial f}{\partial y} \eta + \frac{\partial f}{\partial d_x y} d_x \eta \right). \end{aligned}$$

³In fact, it is possible to extend the concept beyond these limitations, and this will be necessary in quantum physics. This is beyond the scope of this lecture.

⁴An equivalent way of doing so is to take η as some arbitrary function of α , $\alpha\eta(x) = \gamma(\alpha, x)$, and taking only the leading term in a Taylor series in γ .

Inserting this into (5.2) yields

$$\delta F = \delta\alpha \int_{x_1}^{x_2} dx \left(\frac{\partial f}{\partial y} \eta + \frac{\partial f}{\partial d_x y} d_x \eta \right)$$

Dividing by $\delta\alpha$ now defines a functional derivative of F , which for this particular functional yields the right-hand-side. Performing on the right-hand-side further a partial integration on the second term yields

$$\frac{\delta F}{\delta\alpha} = \int_{x_1}^{x_2} dx \eta \left(\frac{\partial f}{\partial y} - d_x \frac{\partial f}{\partial d_x y} \right) + \left. \frac{\partial f}{\partial y} \eta \right|_{x_1}^{x_2},$$

but the last term vanishes, as η vanishes at x_1 and x_2 . Since η is arbitrary, this implies

$$\frac{\delta F}{\delta\alpha} = 0 \Leftrightarrow \frac{\partial f}{\partial y} - d_x \frac{\partial f}{\partial d_x y} = 0,$$

where the equation on f is called the Euler equation. That this has the same form as a single variable-version of the Euler-Lagrange equations for $f = -L$ is already indicating the connection.

The function y which satisfies the Euler equation is therefore the one at which the functional F is stationary, i. e. any small changes in y does not change the value of the functional. Since F maps into the ordinary numbers and is, by assumption, a continuous curve in the trajectories, i. e. a small change in the value of y also creates only a small change in F , this implies that the trajectory y which satisfies the Euler equation extremalizes F , or creates at least a turning point. It is thus equivalent to the integral formulation.

However, which of these conditions is true requires to calculate the second functional derivative of S . Also, there may be more than one extrema or turning point in general. However, as will be seen in the section 5.1.4 already $\delta S = 0$ is sufficient general, so any case will do. This is already hinted at by the fact that the Euler equations of a general functional become for the action the Euler-Lagrange equations. Therefore, any solution to the Euler-Lagrange equations will yield $\delta S = 0$. In practice, most mechanical problems lead to minima of the action, some to a maximum. Turning points play almost never a role.

Before doing so, it is best to study some examples of the procedure. The probably simplest problem is the minimal distance between two points on a plane. While this will comparatively not be mathematically too challenging, this problem introduces the very important concept of a geodesic.

The infinitesimal (Euclidean) distance between two points is given by

$$ds = \sqrt{dx^2 + dy^2},$$

and the total distance between two points is thus

$$S = \int ds = \int \sqrt{1 + \left(\frac{dy}{dx}\right)^2} dx$$

The requirement that this should be the minimal length implies that S now plays the role of F in the general setup, and f is given by

$$f(y, d_x y, x) = \sqrt{1 + \left(\frac{dy}{dx}\right)^2}.$$

The Euler equation is thus

$$\frac{d}{dx} \frac{\partial f}{\partial d_x y} - \frac{\partial f}{\partial y} = \frac{d}{dx} \left(\frac{\frac{dy}{dx}}{\sqrt{1 + \left(\frac{dy}{dx}\right)^2}} \right) = 0$$

It is thus possible to integrate the equation once, yielding, after resolving for the derivative,

$$\frac{dy}{dx} = \sqrt{\frac{c^2}{1 - c^2}} = a,$$

where c is an integration constant. The solution is thus $y = ax + b$, just a straight line. This is the shortest distance between two points in an Euclidean plane. However, this is so because the metric is Euclidean. With the Minkowski metric of chapter 3, the result would be different. Therefore, the shortest connection will be different for different metrics, and the shortest connection is therefore generally called a geodesic.

Another example, this time with further practical use, is the question which is the minimal surface of a flexible object rotating around the z -axis. Since the problem is rotationally symmetric, this problem can be parameterized either using x or y . Choosing x , the surface of a small strip is given geometrically by

$$dA = 2\pi x \times \sqrt{1 + d_x y} dx$$

To find a formulation as an extremal value problem, consider the total surface

$$A[y] = 2\pi \int_{x_1}^{x_2} x \sqrt{1 + d_x y} dx.$$

The corresponding Euler equation is

$$d_x \frac{x d_x y}{\sqrt{1 + (d_x y)^2}} - 0 = 0,$$

since y is cyclic. This is fortunate, and this allows to transform the problem into a first-order differential equation. Integrating with an integration constant a and solving the equation for $d_x y$ yields

$$\frac{dy}{dx} = \frac{a}{\sqrt{x^2 - a^2}},$$

which can be elementary integrated to yield, together with a second constant of integration,

$$y(x) = a \cosh^{-1} \frac{x}{a} + b.$$

Reformulating with initial conditions $y(x_1) = y_1$ and $y(x_2) = y_2$ instead of a and b is, however, not directly possible.

5.1.3 Equivalence to Lagrange's function of the first kind

The equivalence of Hamilton's principle to Lagrange's equation of the second kind is obtained by generalizing the derivation of 5.1.2 to multiple variables y_i (or q_i). This is essentially done by rewriting these functions as

$$y_i = y_{si} + \alpha \eta_i,$$

and thus with the same parameter, but different functions. Then in the remainder it is only necessary to sum over all i , while the rest remains form-invariant, thereby recovering Lagrange equations of the second kind, justifying their name of Euler-Lagrange equations.

It is more complicated to show the equivalence to Lagrange's equation of the first kind, and therefore to lower the condition of non-holonom constraints and the requirement of only a generalized potential rather than a conservative system.

Most steps can actually be performed in the same way, up to

$$\int_{t_1}^{t_2} dt \left(d_t \frac{\partial L}{\partial d_t q_i} - \frac{\partial L}{\partial q_i} \right) \delta q_i = 0.$$

It is not possible to proceed as before, since the variations δq_i are no longer independent. In the same way as in section 4.7 it is possible to add a zero created from the sum of the constraints multiplied by Lagrange multipliers, yielding

$$\int_{t_1}^{t_2} dt \left(d_t \frac{\partial L}{\partial d_t q_i} - \frac{\partial L}{\partial q_i} - \lambda_j f_{ji} \right) \delta q_i = 0$$

Since the added expression is zero, this is still the action, and therefore Hamilton's principle is still valid: Extremalize this expression with respect to the paths. In the same way as in section 4.7 it is possible to use the Lagrange multipliers to eliminate the part of the sum which contains dependent variables. The remainder yields then as Euler equations

$$d_t \frac{\partial L}{\partial d_t q_i} - \frac{\partial L}{\partial q_i} - \lambda_j f_{ji} = 0,$$

together with the determination equations for the Lagrange multipliers and the unresolved constraints. These are again Lagrange's equation of the first kind, which are therefore also equivalent to Hamilton's principle, even with just the ordinary action S - the additional part is only used to resolve the residual dependencies.

5.1.4 Equivalence to d'Alembert's principle

To show that Hamilton's principle is indeed equivalent to d'Alembert's principle it is best to start from (4.4),

$$\sum_i \left(m_i d_t^2 \vec{r}_i - \vec{K}_i \right) \delta \vec{r}_i = 0. \quad (5.3)$$

Though no time elapses during a virtual displacement, the virtual displacements themselves can be different at any time, and therefore are (continuously differentiable) functions of time as well. Furthermore, for the variation of products the same product rule holds as for ordinary differential. Thus

$$\delta \vec{r}_i d_t^2 \vec{r}_i = d_t (\vec{r}_i \delta \vec{r}_i) - (d_t \vec{r}_i) \delta d_t \vec{r}_i = d_t (\delta \vec{r}_i d_t \vec{r}_i) - \frac{1}{2} \delta ((d_t \vec{r}_i)^2). \quad (5.4)$$

It is perfectly permissible to integrate (5.3) after inserting (5.4), yielding

$$0 = \int_{t_1}^{t_2} dt \sum_i \left(d_t (m_i \delta \vec{r}_i d_t \vec{r}_i) - \frac{m_i}{2} \delta ((d_t \vec{r}_i)^2) - \vec{K}_i \delta \vec{r}_i \right) \quad (5.5)$$

The first term is a total derivative and can be integrated directly. However, it vanishes, as the result is proportional to $\delta \vec{r}_i$, which by construction vanishes at t_1 and t_2 .

Transforming the remainder of (5.5) to generalized coordinates yields that the first term is δT . The second term is, for a holonom conservative system,

$$\vec{K}_i \delta \vec{r}_i = Q_i \delta q_i = - \frac{\partial V}{\partial q_i} \delta q_i = -\delta V.$$

Combining yields

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

and thus Hamilton's principle in variational form. Though this was done in forward direction, i. e. starting at d'Alembert's principle and then deriving Hamilton's principle from it, every step is invertible. Thus, Hamilton's principle is as good a starting point to formulate classical mechanics as is d'Alembert's principle.

By virtue of the arguments in section 4.4.4, Hamilton's principle is therefore also equivalent to Newton's laws.

5.1.5 Beyond conservative forces

So far Hamilton's principle only covered conservative cases, or cases in which at least a generalized potential existed. It is possible to extend it even further to include non-conservative cases. For this purpose, define the action as

$$S[q] = \int_{t_1}^{t_2} dt (T + \vec{K}_i \vec{r}_i) \quad (5.6)$$

which is the sum of the kinetic energy and the scalar projected forces, and therefore a well-defined quantity for any mechanical system. If Hamilton's principle should also be true for the non-conservative systems described by this action, it is necessary that the stationary points of this action yield the equations of motion.

Since the technology developed in section 5.1.2 is independent of the mechanics context this only requires to determine the Euler equations for this action, assuming holonom constraints. If the constraints are non-holonom the same procedure as in section 5.1.3 can be used, but with the present integrand rather than the Lagrange function. This yields

$$\begin{aligned} 0 &= d_t \frac{\partial T}{\partial d_t q_i} - \frac{\partial T}{\partial q_i} - Q_i \\ Q_i &= \vec{K}_j \frac{\partial \vec{r}_j}{\partial q_i} \end{aligned}$$

and therefore coincides with the results of section 4.3. As in that case, also here the result simplifies back to the original Euler-Lagrange equations for conservative systems. Especially, in this case $\vec{K}_i \vec{r}_i = -V$.

Thus, Hamilton's principle is in all forms equivalent to Lagrange's equations. Though it has the appeal that all situations are not completely covered, in the form of (5.6) by a single prescription, make the action stationary, in the end it requires again to solve some kind of Lagrange's equation. Thus, though satisfying on conceptual grounds, nothing has yet been gained on practical grounds.

5.2 Phase space and state space

Though the concept of trajectories was extremely useful in reformulating mechanics in a more compact way, it has one essential drawback: It requires to know not only the initial state of a system, but also the final state of a system. Though from a mathematical point of view there is no difference between this requirement and the requirement of knowing position and speed at the initial time, in practice this is often quite different. There, it is usually only known how the system starts, and the question is how it will develop with time. This is especially true when it comes to problems which can no longer be solved in a closed, analytic form. And this is true for almost all systems of interest.

It is therefore useful to reformulate Hamilton's principle as an initial value problem. At first sight, it may seem natural to use the generalized coordinates and speeds for this. But, in fact, it is much more useful to rather use the generalized coordinates and momenta, the latter as defined in (4.18). The reason is that cyclic coordinates imply conserved generalized momenta. Formulating the problem thus in these two quantities will make the whole problem trivial for these directions. Thus, they are advantageous, as no such simple relation exists for the generalized speeds.

Thus, the aim in the following is to reformulate the system in terms of the generalized coordinates and speeds. There are again $2(dn - N)$ of these, thus forming again a space of the same dimensionality. To separate this space from the configuration space before, it is called the phase space.

It is quite useful to reiterate the various concepts of spaces encountered so far.

The basic space is the coordinate space, which has dn coordinates, where d is the number of coordinates and n is the number of involved particles⁵. This can be upgraded to space-time with $dn + 1$ dimensions by adding time. This is true for the effective low-speed system of classical mechanics but for the special relativity version, which both differ by the metric, being either Euclidean or Minkowski, requires an individual time for every particle. However, the time plays a different role than the other coordinates in classical mechanics: Here it parametrizes the trajectories of particle in configuration space. In the relativistic case, this role is played rather by the eigentime.

By introducing generalized coordinates using N holonom constraints, the number of coordinates is reduced to $S = dn - N$. This is the configuration space. The paths of all particles are uniquely described by trajectories in this space. If time is included to characterize the progression along the trajectories, this becomes the $S + 1$ -dimensional event space: Every event is localized at one point in this space.

⁵Systems like fluids without individual particles will be discussed in more detail in section 6.3.

However, both in ordinary space-time as well as in event space it is not sufficient to specify a point to specify a system completely. Even in event space, trajectories may cross. Only by adding generalized speeds the trajectory of a given particle is uniquely determined⁶.

This problem is resolved by the introduction of phase space. By doubling the degrees of freedom by adding the generalized momenta, a $2S$ -dimensional space is obtained. Trajectories do no longer cross. The position along the trajectories can be parametrized by the time. Thus, the position and future movements of any particle of a system is uniquely defined when a position in this space is given. It thus fully describes the state of a system. Conversely, a state is called the minimal collection of information necessary to fully describe a system. Thus, this $2S + 1$ -dimensional space is called the state space⁷. Though the state space has been used to define what a state is in the sense of classical mechanics, any other minimal way is equally good. Also, this concept can be extended to any physical system. E. g., in thermodynamics quantities like temperature and pressure may be part of the minimal information defining a state.

Returning to classical mechanics, this conversely implies that measuring all the minimal information, i. e. determining the point in state space at which a system is located, gives all information about a classical mechanics system⁸. Since a single point is sufficient to fully describe a state this implies that a first-order set of $2S$ differential equations in time should exist which describes the evolution of a state. This will be done in the following, leading ultimately to Hamilton's equations in section 5.4. Lagrange's equation are not yet of this type, as they are second order in time.

⁶That this is sufficient is because Newton's law (2.2), which ultimately underlies any classical mechanics problem, is a differential equation of second order in time. There exists a general mathematical theorem which guarantees that no more initial conditions are needed to uniquely identify a trajectory. If Newton's law would be a third-order differential equation, this would no longer be true, and three initial conditions would be required, and so on. The fact that Newton's law is of second order is nothing which can be derived, but, as noted in section 2.2, is a postulate, derived from observations. Note, however, that there are rare multi-particle systems which are described by higher-order differential equations. However, in these cases this is also only an effective rewriting of initial conditions of multiple particles in the form of a single effective particle.

⁷Consequently, if Newton's law would be rather of m th-order in time, a state space which gives uniquely defined trajectories would be of $mS + 1$ dimensions.

⁸This is the reason why classical mechanics is a deterministic theory. This will no longer be possible in quantum physics.

5.3 Legendre transformations

This is not entirely straightforward. Since the generalized momenta are known as function of the generalized coordinates and speeds, it is possible to invert the various relations to obtain, say, the Lagrange function as a function of the new quantities. But, this problem can be put into a larger context and a general recipe for this type of transformations can be given. In addition to making the procedure more simple for mechanics, the same approach can be used for a wide range of problems, and will play, e. g. again an important role in thermodynamics. This procedure is called Legendre transformation.

To formulate it as generally as possible, consider some function $f(x)$. Later, x will play the role of the generalized speeds and f will be the Lagrange function. The differential of f is

$$df = \frac{df}{dx}dx = udx,$$

where the new variable u will play later the role of the generalized momenta. Having this in mind, the question is how to obtain a function $g(u)$, which is equivalent to f , but now a function of u . Since it appears reasonable that the transformation should be invertible, consider that g is a solution to

$$\frac{dg}{du} = \pm x.$$

Furthermore,

$$df = udx = d(ux) - xdu$$

and therefore

$$\frac{d(f - ux)}{du} = \frac{d(ux) - xdu - (dux)}{du} = -x. \quad (5.7)$$

Thus, the searched for function $g(u)$, the so-called Legendre transformed of $f(x)$, is given by

$$g(u) = f(x) - ux = f(x) - x \frac{df}{dx},$$

which, in principle, solves the problem. At first sight, this seems to be still a function of two variables. What is, of course, necessary, is to still use $df/dx = u$ to reexpress x as a function of u . Note that if $d_x^2 f = 0$ vanishes, a Legendre transformation would not be possible, since u would then not be a variable, but merely a constant.

As all steps can be performed in reverse order, this transformation is reversible. It is noteworthy that just inserting $x(u)$ into f would not be. That is best seen when considering an example. The function

$$f(x) = \alpha x^2 \Rightarrow u = 2\alpha x \Rightarrow x = \frac{u}{2\alpha}$$

Performing an insertion yields

$$f(x(u)) = \alpha \left(\frac{u}{2\alpha} \right)^2 = \frac{1}{4\alpha} u^2,$$

while the Legendre transform is

$$g(u) = f(x(u)) - x(u)u = \frac{1}{4\alpha} u^2 - \frac{u^2}{2\alpha} = -\frac{u^2}{4\alpha}.$$

Consider now the function

$$f'(x) = \alpha(x+c)^2 \Rightarrow u = 2\alpha(x+c) \Rightarrow x = \frac{u}{2\alpha} - c,$$

and thus

$$f'(x(u)) = \alpha \left(\frac{u}{2\alpha} - c + c \right)^2 = \frac{u^2}{4\alpha}.$$

This coincides with the previous case. This type of transformation is therefore not unambiguously invertible. Especially, the result is independent of c , and therefore a continuously infinite number of functions are by this all mapped to the same result. On the other hand, the Legendre transformation is

$$g'(u) = \frac{u^2}{4\alpha} - u \left(\frac{u}{2\alpha} - c \right) = -\frac{u^2}{4\alpha} + uc,$$

which depends on c .

To see that the reverse transformation is indeed unique, consider first the example,

$$\begin{aligned} -x &= d_u g'(u) = -\frac{u}{2\alpha} + c \Rightarrow u = 2\alpha(x+c) \\ f'(x) &= g'(u(x)) + xu(x) = \alpha(x+c)^2. \end{aligned}$$

The reversal of the sign is required to have the corresponding forward and backward transformation. This is seen by considering the full case,

$$f(x) = g(u(x)) + u(x)x = f(x) - u(x)x + u(x)x.$$

The question may arise, what the real significance of the addition is. This shift compensates for the fact that for the inverse transformation is not only necessary to know how the function is modified, but also its derivative. The additional term, as can be seen also from (5.7) ensures that not only the function but also its differential is consistently transformed to the new variables.

Since in the relevant case the function f also depends on more variables, which should not change, it is useful to consider this more general case. If now y plays the role of the additional (mute) general coordinate in $f(x, y)$, the differential takes the form

$$df = \left. \frac{\partial f}{\partial x} \right|_y dx + \left. \frac{\partial f}{\partial y} \right|_x dy = u(x, y)dx + v(x, y)dy.$$

The Legendre transform $g(u, y)$ has then the differential

$$dg = - \left. \frac{\partial g}{\partial u} \right|_y du + \left. \frac{\partial g}{\partial y} \right|_u dy = -x(u, y)du + v(x(y, u), y)dy.$$

Since

$$df = vdy + udx = vdy + d(ux) - xdu$$

implies

$$\begin{aligned} \left. \frac{\partial(f - ux)}{\partial y} \right|_u &= v \\ \left. \frac{\partial(f - ux)}{\partial u} \right|_x &= -x \end{aligned}$$

the desired Legendre transform is given by

$$g(u, y) = f(x(u, y), y) - ux(u, y) = f - x \frac{\partial f}{\partial x}. \quad (5.8)$$

Thus, in the final result the non-transformed variable plays no active role, except that the new variable may depend on it.

5.4 Hamilton's equations

As Lagrange's function is still the basic dynamical quantity, the first step is to apply the Legendre transformation to it. Using the generalized momenta

$$p_i = \frac{\partial L}{\partial \dot{q}_i}$$

yields

$$H(q_i, p_i, t) = p_i \dot{q}_i(q_j, p_j) - L(q_i, p_i(q_j, p_j), t).$$

However, this function is already known. It is Hamilton function (4.25), which coincides under certain conditions, homogeneous kinetic energy of order 2 and a conservative, holonom system, with the total energy $H = T + V$. Though, at that time the generalized momenta was considered as a function of the generalized coordinates and speeds. It will be the Hamilton function which will take over the role of the central quantity from the Lagrange function for most of the rest of this lecture⁹.

After transforming the Lagrange function, the next interesting question is how this affects the equations of motion, especially, what the equivalent reformulation of the Euler-Lagrange equations in phase space are.

⁹As discussed previously, this is different in relativistic systems.

To find them, it is a useful first step to consider the total differential of the Hamilton function,

$$\begin{aligned} dH &= \frac{\partial H}{\partial p_i} dp_i + \frac{\partial H}{\partial q_i} dq_i + \frac{\partial H}{\partial t} dt \\ &= d_t q_i dp_i + p_i dd_t q_i - \frac{\partial L}{\partial q_i} dq_i + \frac{\partial L}{\partial d_t q_i} dd_t q_i - \frac{\partial L}{\partial t} dt = dp_i d_t q_i - \frac{\partial L}{\partial q_i} dq_i - \frac{\partial L}{\partial t} dt, \end{aligned} \quad (5.9)$$

where the terms involving $dd_t q_i$ have canceled because of the definition of the generalized momenta. This can be further simplified by noting that the Euler-Lagrange equations imply

$$d_t p_i = d_t \frac{\partial L}{\partial d_t q_i} = -\frac{\partial L}{\partial q_i}$$

and therefore

$$dH = d_t q_i dp_i - dq_i d_t p_i - \frac{\partial L}{\partial t} dt. \quad (5.10)$$

Comparison of (5.9) and (5.10) yields Hamilton's equations

$$d_t q_i = \frac{\partial H}{\partial p_i} \quad (5.11)$$

$$d_t p_i = -\frac{\partial H}{\partial q_i} \quad (5.12)$$

$$-\frac{\partial L}{\partial t} = \frac{\partial H}{\partial t}, \quad (5.13)$$

which are the new equations of motion determining the dynamics as the Euler-Lagrange equations did before. They are also called canonical equations. The last equation is actually not a real equation of motion, but rather a consistency condition, as it is not an equation involving a separate variable. The equations (5.11-5.12) are first order in time, and are therefore describing the evolution of a state in state space with knowledge of a single point, as was aimed at in section 5.2.

The most remarkable result is that Hamilton's equations are now first-order differential equations, rather than the second-order differential equations of Lagrange. In practice, first-order equations are usually easier to solve, and therefore Hamilton's equations are technically a step forward. The disadvantage is that the number of equations of motion to be solved has doubled, but in practice this is still better¹⁰. The result when solving these equations is then no longer a trajectory in configuration space, but rather a trajectory in phase space.

¹⁰Note that ordinary differential equations of second order can always be rewritten as a set of twice as much first-order differential equations. This is not necessarily so for partial differential equations as the equations of motion are. The result is therefore not trivial on mathematical grounds.

Though in general the Hamilton function is the Legendre transform of the Lagrange function, under certain conditions discussed in section 4.8.1, it is just the total energy of the system, $H = T + V$. This rather simple relation to the Lagrange function $L = T - V$ comes about as this is true if the kinetic energy is at most quadratic in the speeds. Then the first term in the Legendre transformation taking care of the differential properties is $2T$, and therefore $H = 2T - T + V = T + V$ is the total energy. Though this is the most relevant case, this is by far not always the case.

Similar as there, it can be shown that

$$d_t H = \frac{\partial H}{\partial q_i} d_t q_i + \frac{\partial H}{\partial p_i} d_t p_i + \partial_t H = \frac{\partial H}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial H}{\partial q_i} + \partial_t H = \partial_t H.$$

Here, Hamilton's equations of motions (5.11-5.12) have been used. This implies that if the Hamilton function is not explicitly depending on time, $\partial_t H = 0$, it is a conserved quantity, and actually constant as a function of time. Thus, the time-dependencies of the q_i and p_i have to cancel each other inside the Hamilton function in this case. If the Hamilton function coincides with the energy, the energy is in this case conserved.

Furthermore, because of (5.12) any cyclic coordinate in the Lagrange function is necessarily also cyclic in the Hamilton function. In case of a cyclic coordinate this also implies that one of Hamilton's equations of motion is solved trivially. The actual value of the corresponding generalized coordinate is then determined by the initial conditions. This is quite different from the Lagrange case, as the Lagrange function depends on the generalized speeds rather than the generalized momenta, and therefore the existence of a cyclic coordinate does not immediately solve any of the equations of motion. This is again a practical advantage of the Hamilton formalism over the Lagrange formalism.

The disadvantage, stated without proof here, of the Hamilton formalism is that it is more complicated in the relativistic case. Therefore, as a compromise, the so-called Routh formalism performs the Legendre transformation only for cyclic coordinates. The resulting function is then still of the Lagrange type, but depends for s cyclic coordinates only on the q_1, \dots, q_n and the $n - s$ generalized speeds $d_t q_{s+1}, \dots, d_t q_n$, and thus creates only $n - s$ second-order differential equations and $2s$ first-order differential equations. As this formalism plays essentially no role in quantum physics, and only in very special cases in classical mechanics, it will not be developed here further.

Note that (5.11) implies that if a generalized momentum is cyclic, then the corresponding coordinate is constant as well. This case is, however, much rarer than that of a cyclic coordinate.

It is quite useful to study the procedure from the original system up to Hamilton's equations and the solution of Hamilton's equations for an example. To facilitate the

comparison to previous results, this will be the harmonic oscillator, though Hamilton's formalism is overkill for it.

In this case, there is a single generalized coordinate $q = x$ describing the position of the oscillator. The kinetic and potential energy of this conservative system is

$$\begin{aligned} T &= \frac{m}{2}(d_t q)^2 \\ V &= \frac{k}{2}q^2. \end{aligned}$$

This yields the Lagrange function

$$L = T - V = \frac{m}{2}(d_t q)^2 - \frac{k}{2}q^2,$$

in which no coordinate is cyclic. However, it does not depend explicitly on the time, and therefore the energy will be conserved. The generalized momentum is

$$p = \frac{\partial L}{\partial d_t q} = m d_t q.$$

The Legendre transformation yields the Hamilton function

$$H = p d_t q - L(q, d_t q(q, p)) = \frac{p^2}{m} - \frac{1}{2m}p^2 + \frac{k}{2}q^2 = \frac{1}{2m}p^2 + \frac{k}{2}q^2 = T + V,$$

which coincides with the conserved energy. This could be used to eliminate either q or p . But it is more instructive to use Hamilton's equations (5.11-5.12), being

$$\begin{aligned} d_t q &= \frac{\partial H}{\partial p} = \frac{p}{m} \\ d_t p &= -\frac{\partial H}{\partial q} = -kq \end{aligned}$$

This set of equations can be solved in multiple ways. Either, it is possible to replace p or q by using the conserved total energy, or by inserting one equation into the other, yielding again a second-order differential equation. At any rate, the solutions are

$$\begin{aligned} q(t) &= q_0 \sin\left(\frac{k}{m}t + \phi_0\right) \\ p(t) &= \frac{mq_0}{k} \cos\left(\frac{k}{m}t + \phi_0\right), \end{aligned}$$

with the two integration constants. The total energy is

$$H = E = \frac{kq_0^2}{2} \cos^2\left(\frac{k}{m}t + \phi_0\right) + \frac{kq_0^2}{2} \sin^2\left(\frac{k}{m}t + \phi_0\right) = kq_0^2.$$

Thus, the energy is completely determined by the initial conditions. The trajectory in phase space is a closed ellipsoid, where the relative size of the major axes depends on the initial conditions as well.

Such a closed path in phase space is typical for periodic systems. If the path is not closed, but both the coordinates as well as the generalized momenta are bounded, this is called an aperiodic system.

5.5 Action principles

With the introduction of the phase space, it is possible to reformulate the action principles of section 5.1. Each of the following reformulation puts emphasis on a different aspect of a mechanical system. They therefore center the discussion on different concepts. Likewise, depending on the knowledge about a system, different of these principles may be useful in practical applications.

5.5.1 Modified Hamilton's principle

The first, perhaps obvious, modification is to change from a formulation in terms of trajectories in configuration space to one in phase space. The question is thus, what is the characteristic property of a phase space trajectory to be the solution of a mechanical problem. In the configuration space case it was that it extremalized the action.

It is therefore reasonable to start by reformulating the action in phase space. To do so, the Lagrange function in (5.1) is replaced by the Hamilton function using the inverse Legendre transformation, yielding

$$S[q, p] = \int_{t_1}^{t_2} dt (p_i d_t q_i(q_j, p_j) - H(q_k, p_k)),$$

which is thus a functional of the phase space trajectory. Still, the variation under a change of the trajectory in configuration space must vanish. An important insight is that the initial conditions in (5.1) only required that the variations of q_i and $d_t q_i$ vanish at t_1 and t_2 . This does not necessarily imply that any variation of the generalized momenta do vanish at t_1 and t_2 , as long as the variations of the generalized coordinates and speeds vanish. Thus, $p_i(t) = p_i(t) + \alpha \omega_i(t)$ with $\omega(t_1)$ and $\omega(t_2)$ not constrained in general.

Performing the variation as in 5.1.2 yields

$$\delta S = \delta \alpha \int_{t_1}^{t_2} dt \left(\omega_i d_t q_i + p_i d_t \eta_i - \frac{\partial H}{\partial q_i} \eta_i - \frac{\partial H}{\partial p_i} \omega_i \right).$$

Performing a partial integration

$$\int_{t_1}^{t_2} dt p_i d_t \eta_i = p_i \eta_i \Big|_{t_1}^{t_2} - \int_{t_1}^{t_2} dt \eta_i d_t p_i = - \int_{t_1}^{t_2} dt \eta_i d_t p_i$$

yields

$$0 = \frac{\delta S}{\delta \alpha} = \int_{t_1}^{t_2} dt \left(\omega_i \left(d_t q_i - \frac{\partial H}{\partial p_i} \right) - \eta_i \left(d_t p_i + \frac{\partial H}{\partial q_i} \right) \right).$$

Given that the variations η and ω are independent and arbitrary, this will only vanish if Hamilton's equations (5.11-5.12) are fulfilled. Conversely, this implies that the physical trajectories in phase space extremalize the action. Thus, the physical trajectories in both configuration space and phase space extremalize the action.

5.5.2 Maupertius' action principle

A different formulation is due to Maupertius. While it is in spirit similar to Hamilton's principles, it operates on a different concept of variations. It is applicable for conservative systems only, and thus systems in which the Hamilton function is a constant of motion.

It is based on a different action formulation,

$$A = \int_{t_1}^{t_2} dt p_i d_t q_i. \quad (5.14)$$

and considers the following type of trajectory variation: Rather than keeping the time constant for all admissible trajectories, this principle requires that the Hamilton function has the same value for every trajectory. This is the reason why it only makes sense for conservative systems. Also, the trajectories should be compatible with the initial conditions, i. e. start at the same points and end at the same points. Trajectories from the configuration space may be admissible for both, either, or none of these variations.

As a consequence, it is necessary to also consider that the time changes for a trajectory variation, $t \rightarrow t + \alpha \tau$. To make this sensible, every trajectory can be considered to be parameterized by a parameter s , where $t(s) + \alpha \tau(s)$ is a (strictly) monotonously increasing function of s . Therefore, a variation of a trajectory now takes the form

$$\Delta q = \Delta \alpha (\eta + \tau d_t q) = \Delta \alpha (\delta q + (d_t q) \Delta t),$$

and the symbol Δ is used to make the distinction between the two types of variations explicit. Due to the explicit occurrence of the time, this type of variation no longer

commutes with the total time derivative,

$$d_t \Delta q = \Delta \alpha(d_t \delta q + d_t((d_t q) \Delta t)) = \Delta \alpha(\delta d_t q + (d_t^2 q) \Delta t + d_t q d_t \Delta t) \neq \Delta \alpha(\delta d_t q + (d_t^2 q) \Delta t) = \Delta d_t q.$$

This statement holds true for any such variation. Especially, for an arbitrary function of the coordinates

$$\frac{\Delta f(q, t)}{\Delta \alpha} = \frac{\partial f}{\partial q} \Delta q + \frac{\partial f}{\partial t} \Delta t = \frac{\partial f}{\partial t} (\delta q + (d_t q) \Delta t) + \frac{\partial f}{\partial t} \Delta t = \delta f + (d_t f) \Delta t. \quad (5.15)$$

Especially, since neither p nor $d_t q$ are further constrained, their variations have to be calculated in this way.

Varying now the action A yields

$$\Delta A = \Delta \int_{t_1}^{t_2} dt p_i d_t q_i = \Delta \int_{t_1}^{t_2} dt (L + H) = \Delta \left(\int_{t_1}^{t_2} dt L + H(t_2 - t_1) \right) = \Delta \int_{t_1}^{t_2} dt L + H(\Delta t_2 - \Delta t_1),$$

where it has been used that by construction H is constant along all admitted trajectories. Since a time derivative and a variation Δ do not commute, so neither does a time integration and the variation. However, the integrals are functionals of the trajectories, and therefore (5.15) can be used. This yields

$$\Delta A = \delta S + (d_{t_2} - d_{t_1}) \int_{t_1}^{t_2} dt L \Delta t + H(\Delta t_2 - \Delta t_1) = \delta S + (L + H) \Delta t \Big|_{t_1}^{t_2},$$

where the boundary term appears as the consequence of varying t_1 and t_2 , which are no longer fixed. Unfortunately, the first term does not vanish, as it does only so for trajectories of fixed time, but not of fixed Hamilton function. It is therefore necessary to calculate it, using that this variation still commutes with time derivatives, yielding

$$\begin{aligned} \int_{t_1}^{t_2} dt \delta L &= \int_{t_1}^{t_2} dt \left(\frac{\partial L}{\partial q_i} \delta q_i + \frac{\partial L}{\partial d_t q_i} d_t \delta q_i \right) = \int_{t_1}^{t_2} dt d_t \left(\frac{\partial L}{\partial d_t q_i} \delta q_i \right) \\ &= \left. \frac{\partial L}{\partial d_t q_i} \delta q_i \right|_{t_1}^{t_2} = \left(\frac{\partial L}{\partial d_t q_i} \Delta q_i - \frac{\partial L}{\partial d_t q_i} (d_t q_i) \Delta t \right) \Big|_{t_1}^{t_2}. \end{aligned}$$

where in the third step the Euler-Lagrange equations and in the last step (5.15) has been used. Since the initial conditions remain valid, $\Delta q_i(t_1) = \Delta q_i(t_2) = 0$, and the first term drops out. Recognizing the generalized momenta in the second term and combining everything yields

$$\Delta A = (L - p_i d_t q_i + H) \Delta t \Big|_{t_1}^{t_2} = 0,$$

for any Δt , since this is just the definition of the Hamilton function. Thus, every trajectory satisfying the Hamilton principle will also satisfy this minimal action principle.

While this formulation of the action principle is not outright useful, its important message is that the partition of trajectories in configuration space used before is not the only possibility to formulate classical mechanics. At the same time, it emphasizes that the selection criterion of trajectories still needs to be tied to some physical concept characteristic of classical mechanics.

It should be noted that in most of the remaining lecture the name action refers to (5.1) if not remarked otherwise.

5.5.3 Fermat's principle

Another reformulation of the action is the one of Fermat. It is this principle which lends itself particularly well to generalization of an action principle to optics, quantum physics, and (general) relativity. However, in classical mechanics it is less useful, as it is a very special case. The following is therefore again of particular interest only for its conceptual implications.

Consider a further specialization, in which V is also constant, implying that the kinetic energy needs to be constant as well. This implies that the integration kernel of (5.14) is, due to

$$2T = H + L = p_i dq_i = c$$

constant itself. Thus

$$\Delta A = \Delta \int_{t_1}^{t_2} dt c = c \Delta(t_2 - t_1),$$

which must vanish. This implies that the trajectory is chosen which extremalizes the variation of the time difference, and thus which makes the traveling time extremal, usually minimal. This is Fermat's principle, also known as the principle of soonest arrival. In geometrical optics it is the same underlying principle which requires the light to take the shortest, and thus in a fixed medium fastest, path. This equivalence is also true for a force-free particle, which implies constant speed dx/dt , and therefore

$$0 = \Delta \int_{t_1}^{t_2} \frac{dx}{dt} dt = \Delta \int_{x_1}^{x_2} dx, \quad (5.16)$$

and thus the requirement to extremalize the path, usually making it as short as possible. Though trivial in mechanics, the concept generalizes, as noted above. The path of shortest

length, which is a solution to a given problem, has therefore a special name: It is called again a geodesic.

5.5.4 Jacobi's principle

A further important concept is introduced when any explicit appearance of the time is eliminated from the action principle. Start again from (5.14). This time the potential is not constant, but still for a conservative system

$$0 = \Delta \int_{t_1}^{t_2} dt p_i d_t q_i = \Delta \int_{t_1}^{t_2} dt (H + L) = \Delta \int_{t_1}^{t_2} dt 2T$$

applies. If the constraints are skleronom, then

$$T = \sum_i m_i (d_t r_j^i)^2 = \sum_{ijkl} m_i \frac{\partial r_j^i}{\partial q_k} \frac{\partial r_j^i}{\partial q_l} (d_t q_k)(d_t q_l) = \sum_{kl} \mu_{kl} (d_t q_j)(d_t q_l),$$

where the quantity

$$\mu_{jl} = \sum_{ij} m_i \frac{\partial r_j^i}{\partial q_k} \frac{\partial r_j^i}{\partial q_l},$$

though being a function of the q_i is sometimes called generalized mass. It is, however, better known as the configuration space metric. This is best seen by multiplying the expression by dt^2 , yielding

$$(dr)^2 = \sum_{ij} m_i dr_j^i dr_j^i = \sum_{kl} \mu_{kl} dq_j dq_l = (d\rho)^2$$

Thus, the generalized metric transforms a length element in coordinate space to configuration space. Formally, the (diagonal) matrix of masses can be considered also as such a metric.

This reformulates the action as

$$0 = \Delta \int_{t_1}^{t_2} dt 2T = \Delta \int_{t_1}^{t_2} 2T \frac{dt}{d\rho} d\rho = \Delta \int_{\rho_1}^{\rho_2} 2T \frac{\sqrt{2T}}{d} \rho = \Delta \int_{\rho_1}^{\rho_2} \sqrt{E - V} d\rho.$$

The final expression does no longer involve the time, and is thus the searched-for expression. This reformulation of the action principle is known as Jacobi's principle. If $V = 0$, the energy is constant, and the principle turns into

$$0 = \Delta \int_{\rho_1}^{\rho_2} d\rho.$$

This is a reformulation of Fermat's principle (5.16) in configuration space: In the absence of forces, the system moves along a geodesic in configuration space. One interesting consequence of this principle is that, because the time no longer appears, the Δ -type and δ -type variations again coincide.

While the principle is useful in itself, just remember planetary motions where the solution in section 2.7.3 in terms of the time is extremely complicated but without is straightforward, it is the concept of the metric in configuration space which also deserves attention.

To illustrate the metric, first consider the trivial case of the generalized coordinate being just the ordinary ones for a single particle. Then

$$\mu_{kl} = m \frac{\partial x_i}{\partial q_k} \frac{\partial x_i}{\partial q_l} = m \delta_{ik} \delta_{il} = m \delta_{kl},$$

and the metric is only a rescaled unit matrix. A little less trivial is the case where the generalized coordinates are the spherical coordinates (4.19-4.21). The metric is then the matrix, using $q_1 = r$, $q_2 = \theta$, $q_3 = \phi$,

$$\mu = m \begin{pmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & r^2 \sin^2 \theta \end{pmatrix}$$

and thus still a diagonal matrix.

An intriguing example for the Jacobi principle is that of electron deflection. Consider two materials, in which an electron moves under the influence of a constant (electrostatic) potential, but where these potentials differ between both media, say V_1 in medium 1 and V_2 in medium 2. Thus, the potential is constant, except at the interface, where it jumps. Since a single path is investigated, it is always possible to put everything in the x - y -plane. Now let the electron start somewhere in the first medium at the position 1, hit the interface at some point 2, and finally end up in the second medium at position 3. The interface should be located along the x -axis at $y = 0$. Since there are no forces in the two media acting, as the potential is constant, the movement in the individual media is that of a free particle.

The Jacobi principle the requires

$$\begin{aligned} 0 &= \Delta \int_1^3 \sqrt{2m(E - V)} \sqrt{dx^2 + dy^2} \\ &= \Delta \int_1^2 \sqrt{2m(E - V_1)} \sqrt{dx^2 + dy^2} + \Delta \int_2^3 \sqrt{2m(E - V_2)} \sqrt{dx^2 + dy^2} \end{aligned}$$

Since the energy and the potentials V_i are constant, they can be moved outside the integral. Then the free movement in the medias imply

$$0 = \sqrt{2m(E - V_1)}\Delta\sqrt{x_2^2 + y_1^2} + \sqrt{2m(E - V_2)}\Delta\sqrt{(x_2 - x_3)^2 + y_3^2},$$

where it was chosen that $x_1 = 0$. Since, as noted, time plays no role in the variation, (5.15) implies

$$0 = \left(\sqrt{2m(E - V_1)}d_{x_2}\sqrt{x_2^2 + y_1^2} + \sqrt{2m(E - V_2)}d_{x_2}\sqrt{(x_2 - x_3)^2 + y_3^2} \right) \delta x$$

The variation δx is non-zero, and can therefore be divided by. This yields

$$\begin{aligned} & \sqrt{(E - V_1)}\frac{x_2}{\sqrt{x_2^2 + y_1^2}} - \sqrt{(E - V_2)}\frac{x_3 - x_2}{\sqrt{(x_3 - x_2)^2 + y_3^2}} \\ &= \sqrt{(E - V_1)}\sin\alpha - \sqrt{(E - V_2)}\sin\beta. \end{aligned}$$

Therefore, the deflection of the electron at the surface is given by

$$\frac{\sin\alpha}{\sin\beta} = \sqrt{\frac{E - V_2}{E - V_1}} = \frac{|v_2|}{|v_1|},$$

and is determined by the electron's speed in both media. This does not incidentally look like the refraction law of optics, as this can be derived in a very similar way from Jacobi's principle applied to geometrical optics.

5.6 Covariant Hamiltonian mechanics

With the action principles a point has been reached where the attempt can be made to give a formulation compatible with special relativity.

5.6.1 Formulation

The basis for this will be Hamilton's principle in its integral and variational formulation. Again, the formulation is postulated, and its equivalence to (3.9) will be shown afterwards.

To have a genuine relativistic formulation, the best starting point is to start with a Lorentz scalar to encode the physics. As the Lagrange function has already been a scalar under rotation, it is natural to require that the Lagrange function becomes also a Lorentz scalar. It then needs to depend on Lorentz vectors, rather than ordinary vectors, as generalized coordinates,

$$L = L(x_\mu, u_\mu, \tau),$$

where x_μ is the position of the particle, u_μ is its four-velocity, and τ is the eigenzeit. Of course, it is possible to also introduce generalized coordinates or add more particles, but this will not be done here.

It is then possible to use the eigenzeit τ to define an action as

$$S = \int_{\tau_1}^{\tau_2} L(x_\mu, u_\mu, \tau) d\tau, \quad (5.17)$$

which therefore acts again on trajectories. After all, the eigenzeit was introduced as a parameter describing the trajectory, and not withstanding its physical interpretation it is not part of the coordinates. Especially, here also $t(\tau)$, and thus there are now four components of the trajectory.

From the point of view of mathematics, this just introduces another variable, and therefore the arguments of section 5.1.2 can be repeated identically, leading to the relativistic form of the Euler-Lagrange equation

$$\frac{d}{d\tau} \frac{\partial L}{\partial u_\mu} - \frac{\partial L}{\partial x_\mu} = 0, \quad (5.18)$$

giving four partial differential equations for the four unknown quantities $x_\mu(\tau)$. Hamilton's principle is then defined in the same way as before: An integral over the Lagrange function, and the variation with respect to the trajectories, which are now worldlines.

To show that this is equivalent to the, also postulated, relativistic form of Newton's law, start first with the case of a free particle.

5.6.2 Point particle

Take a particle moving along its world line. Classically, a trajectory is described by the 3 spatial coordinates $x_i(t)$ as a function of time $t = x_0$. Now there is the world-line with 4 functions $X_\mu(\tau)$ of the eigenzeit. For the following it is important to note that the eigenzeit strictly monotonously increases along the world-line.

It is now postulated that a free particle of mass m is described by the action

$$S_{pp} = -m \int d\tau \sqrt{-\partial_\tau X^\mu \partial_\tau X_\mu}. \quad (5.19)$$

Performing the variation along the world line

$$\delta \dot{X}_\mu \equiv \delta \partial_\tau X^\mu = \partial_\tau \delta X^\mu$$

yields the equation of motion as

$$\begin{aligned}
\delta S_{pp} &= -m \int d\tau \left(\sqrt{-\dot{X}_\mu \dot{X}^\mu} - \sqrt{-\left(\dot{X}^\mu + \delta \dot{X}^\mu\right) \left(\dot{X}_\mu + \delta \dot{X}_\mu\right)} \right) \\
&= -m \int d\tau \left(\sqrt{-\dot{X}_\mu \dot{X}^\mu} - \sqrt{-\left(\dot{X}_\mu \dot{X}^\mu + 2\dot{X}^\mu \delta \dot{X}_\mu\right)} \right) \\
&= -m \int d\tau \left(\sqrt{-\dot{X}_\mu \dot{X}^\mu} - \sqrt{-\dot{X}_\mu \dot{X}^\mu \left(1 + 2\frac{\dot{X}^\rho \delta \dot{X}_\rho}{\dot{X}_\nu \dot{X}^\nu}\right)} \right) \\
&\stackrel{\text{Taylor}}{=} m \int d\tau \frac{\dot{X}^\mu \delta \dot{X}_\mu}{\sqrt{-\dot{X}^\nu \dot{X}_\nu}}
\end{aligned}$$

where in the last line use has been made of the infinitesimal smallness of $\delta \dot{X}_\mu$ and the square root has been Taylor-expanded.

Defining now the four-speed as

$$u^\mu = \frac{\dot{X}^\mu}{\sqrt{-\dot{X}_\nu \dot{X}^\nu}}$$

yields the equation of motion after imposing the vanishing of the action under the variation and a partial integration as

$$m \dot{u}^\mu = 0$$

This is nothing else then the equation of motion for a free relativistic particle, which of course reduces to the one of Newton in the limit of small speeds. This also justifies the interpretation of m as the rest mass of the particle. Note the fact that the division done just normalizes the four-speed, as the length of $d_\tau x_\mu$ is a constant, as discussed in section 3.3.

With τ the eigentime the action is indeed Poincare-invariant. This can be seen as follows. A Poincare transformation is given by

$$X'^\mu = \Lambda^\mu_\nu X^\nu + a^\mu.$$

Inserting this expression for the argument of the square root yields

$$\partial_\tau (\Lambda^\mu_\nu X^\nu + a^\mu) \partial_\tau (\Lambda^\omega_\mu X_\omega + a^\mu) = (\Lambda^\mu_\nu \Lambda^\omega_\mu) \partial_\tau X^\nu \partial_\tau X_\omega.$$

Since the expression in parenthesis is just δ^ω_ν because of the (pseudo-)orthogonality of Lorentz transformations, this makes the expression invariant. Since the eigentime is invariant by definition, this shows the invariance of the total action.

Additionally, it is also reparametrization invariant, i. e., it is possible to transform the eigentime to a different variable without changing the contents of the theory, as it ought to be: Physics should be independent of the coordinate systems imposed by the observer. This is what the equivalence principle is about. It is instructive to study this in more detail.

To show this invariance for the action (5.19) take an arbitrary (but invertible) reparametrization $\tau' = f(\tau)$. This implies

$$\begin{aligned}\dot{\tau}' &= \frac{d\tau'}{d\tau} \\ d\tau &= \frac{d\tau'}{\dot{\tau}'},\end{aligned}$$

yielding the transformation property of the integral measure. For the functions follows then

$$\dot{X}^{\mu'}(\tau') = \dot{X}^{\mu}(\tau) \frac{d\tau}{d\tau'} = \dot{X}^{\mu} \frac{1}{\dot{\tau}'}$$

Hence the scalar product changes as

$$\dot{X}^{\mu'} \dot{X}_{\mu'} = \frac{1}{\dot{\tau}'^2} \dot{X}^{\mu} \dot{X}_{\mu}.$$

One power of $\dot{\tau}'$ is removed by the square root, and the remaining one is then compensated by the integral measure.

Showing this explicitly for the action (5.19) was rather tedious, and it is useful to rewrite the action. For this purpose it is useful to introduce a metric along the world line. Since the world line is one-dimensional, this metric is only a single function $\gamma_{\tau\tau}(\tau)$ of the eigentime. This yields a trivial example of a so-called tetrad η , which is defined as

$$\eta(\tau) = (-\gamma_{\tau\tau}(\tau))^{\frac{1}{2}}.$$

The quantity $\gamma_{\tau\tau}$ is called the world-line metric, as it will be found to measure distances along the world-line.

For the moment, consider the tetrad as an independent function in a new action defined as

$$S'_{pp} = \frac{1}{2} \int d\tau \left(\frac{\dot{X}^{\mu} \dot{X}_{\mu}}{\eta} - \eta m^2 \right).$$

Under a reparametrization $\tau \rightarrow \tau'(\tau)$ it is defined that the functions X and η transform as

$$\begin{aligned}X(\tau) &= X(\tau'(\tau)) \\ \eta'(\tau') &= \eta(\tau) \frac{d\tau}{d\tau'} = \frac{1}{\dot{\tau}'} \eta(\tau)\end{aligned}\tag{5.20}$$

The transformation of η (5.20) takes care of the extra factor of $\dot{\tau}'$, and also makes the second expression invariant.

To show that the new action is indeed equivalent to the old, and that η is thus just an auxiliary function, can be shown by using the equation of motion for η . Using the Euler-Lagrange equation this yields

$$\begin{aligned} 0 = \frac{d}{d\tau} \frac{\partial L}{\partial \dot{\eta}} - \frac{\partial L}{\partial \eta} &= \frac{\dot{X}^\mu \dot{X}_\mu}{\eta^2} + m^2 \\ \implies \eta^2 &= -\frac{\dot{X}^\mu \dot{X}_\mu}{m^2}. \end{aligned}$$

Thus knowledge of X determines η completely, since no derivatives of η appear. The tetrad η is a so-called auxiliary function. Inserting this expression into (5.20) leads to

$$\begin{aligned} S'_{pp} &= \frac{1}{2} \int d\tau \left(\frac{\dot{X}^\mu \dot{X}_\mu}{\sqrt{-\frac{\dot{X}^\nu \dot{X}_\nu}{m^2}}} - \sqrt{-\frac{\dot{X}^\mu \dot{X}_\mu}{m^2}} m^2 \right) \\ &= \frac{m}{2} \int d\tau \left(-\frac{\dot{X}^\mu \dot{X}_\mu}{\sqrt{-\dot{X}^\nu \dot{X}_\nu}} - \sqrt{-\dot{X}^\mu \dot{X}_\mu} \right) \\ &= -m \int d\tau \sqrt{-\dot{X}^\mu \dot{X}_\mu} = S_{pp}. \end{aligned}$$

Thus S'_{pp} is indeed equivalent to S_{pp} . But, there is an additional advantage. By separation of the mass S'_{pp} can also be applied to the case of $m = 0$ directly, which is only possible in a limiting process for the original action S_{pp} .

Studying now (5.18) makes also clear why Newton's law in special relativity, (3.9), cannot so easily be derived. Because the fourth component of the relativistic force depends on the speed, this requires in general a delicate cancellation between the first and second term in (5.18) to work. This is in contrast to the classical case, where the force is just produced from the second term. This problem will therefore not be study in general further here.

5.7 Canonical transformations

One of the important insights in chapter 4 was that in section 4.5 it was shown that the formulation using Lagrange's equations is invariant of the particular chosen coordinates. The formulation of mechanics in terms of Hamilton's principle gives this a conceptual more important interpretation. Since the objects are now trajectories, rather than the generalized coordinates and speeds, the coordinate-system-invariance is the statement that

it does not matter how the trajectories are described. The actual dynamical objects of mechanics are the trajectories, not the coordinates.

The introduction of Hamilton's equations requires to reinvestigate these statements. The question is, whether the trajectories in coordinate space can be replaced by states, and thus whether Hamilton's equations are form-invariant under changes of the so-called canonical coordinates of generalized coordinates and momenta. However, this does not require any deep calculations. When changing the generalized coordinates and speeds to new ones Q and $d_t Q$, which are arbitrary invertible and continuously differentiable functions of time, and reexpressing the Lagrange function in these new coordinates, it was already shown in (4.5) that the equations of motion remain form-invariant. Defining thus new generalized momenta as

$$P_i = \frac{\partial L}{\partial d_t Q_i}, \quad (5.21)$$

the same derivation of Hamilton's equation can be performed as before, exploiting the form-invariance of the Euler-Lagrange equations, and thus arriving at the same form of Hamilton's equations (5.11-5.13), but now for the new coordinates.

Furthermore, in section 4.5 it was shown that it is possible to add to the Lagrange function a total time derivative of a function depending only on the generalized coordinates and time, (4.17), and this left the Euler-Lagrange equations also untouched. This has a somewhat different impact in Hamilton's formulation. Deriving from (4.17) the generalized momenta yields

$$p_i^f = \frac{\partial(L + d_t f)}{\partial d_t q_i} = \frac{\partial L}{\partial d_t q_i} + \frac{\partial}{\partial d_t q_i} \left(\partial_t f + \frac{\partial f}{\partial q_j} d_t q_j \right) = p_i + \frac{\partial f}{\partial q_i}. \quad (5.22)$$

That is, adding such a function changes the generalized momenta, while the generalized coordinates remain unchanged, $q_i^f = q_i$. This changes the Hamilton function as

$$H^f = p_i^f d_t q_i^f - L^f = p_i^f d_t q_i^f - L - d_t f = p_i d_t q_i - L + d_t q_i \frac{\partial f}{\partial q_i} - \partial_t f - \frac{\partial f}{\partial q_i} d_t q_i = H - \partial_t f.$$

Thus, while the Lagrange function is shifted by a total derivative, the Hamilton function is shifted by a partial derivative. The canonical equations take the form

$$\begin{aligned} \frac{\partial H^f}{\partial p_i^f} &= \frac{\partial H(q_k, p_k^f, t)}{\partial p_i^f} = \frac{\partial H}{\partial p_j} \frac{\partial p_j}{\partial p_i^f} = \delta_{ij} \frac{\partial H}{\partial p_j} = \frac{\partial H}{\partial p_i} = d_t q_i = d_t q_i^f \\ \frac{\partial H^f}{\partial q_i^f} &= \frac{\partial(H(q_i, p_i^f, t) + \partial_t f)}{\partial q_i} = \frac{\partial H}{\partial q_i} - \frac{\partial^2 f}{\partial t \partial q_i} + \frac{\partial H(q_k, p_k^f, t)}{\partial p_j^f} \frac{\partial p_j^f}{\partial q_i} \\ &= \frac{\partial H}{\partial q_i} - \frac{\partial^2 f}{\partial t \partial q_i} + (d_t q_j) \frac{\partial^2 f}{\partial q_j \partial q_i} = -d_t p_i - d_t \frac{\partial f}{\partial q_i} = -d_t p_i^f. \end{aligned}$$

Thus, the equations are indeed also form-invariant.

While this result is in itself not totally surprising, as the Lagrange and the Hamilton formalism are for any sets of coordinates equivalent as discussed above, this result has some far-reaching consequences. It implies that it is possible to locally redefine the generalized momenta, i. e. change the generalized momenta at every point in space and time almost arbitrarily, and still get the same physics. At the same time, the trajectories remain fixed, as the generalized coordinates do not change: The particle still move in the same way. And also with the same speed, as also the generalized speeds are not changed. This implies that the generalized momenta are not unique, but can be changed locally. This is a much stronger statement as a change of coordinate system, as this is done for all coordinates in the same way, it is global. This arbitrariness implies that some of the information contained in the generalized momenta is arbitrary. This is not a surprise. As noted above, the basic object is the trajectory. Any solution with the same trajectory will provide the same physics. In the Lagrange formulation, this arbitrariness is not there, as the generalized speeds are uniquely determined once the trajectories are known. This is, as seen here, not true for the generalized momenta.

Such a local arbitrariness is also known as a gauge freedom. Its generalization plays a very important role in physics. Why this is the case can already be seen for the present case in classical mechanics.

This freedom implies that the possible redefinitions of variables in the Hamilton case is much larger than in the Lagrange case. There it was only possible to change the generalized coordinates and speeds in a way which maintained the fact that the generalized speeds were derivatives of the generalized coordinates. Here, there is more freedom. And this freedom can be used to simplify problems. That is the idea behind the following concept.

While it was straightforward than any transformation changing generalized coordinates and speeds left Hamilton's equations invariant, this is actually not possible for an invertible and differentiable point transformation of generalized coordinates and momenta¹¹

$$Q_i = Q_i(q_j, p_j, t) \quad (5.23)$$

$$P_i = P_i(q_j, p_j, t). \quad (5.24)$$

Point transformations, which satisfy some Hamilton function's $h(Q_i, P_i, t)$ Hamilton's

¹¹Note that the P_i do not necessarily fulfill the relation (5.21). It will be necessary to specify the conditions on the point transformation when this is the case.

equations

$$d_t Q_i = \frac{\partial h(Q_i, P_i, t)}{\partial P_i} \quad (5.25)$$

$$d_t P_i = -\frac{\partial h(Q_i, P_i, t)}{\partial Q_i} \quad (5.26)$$

are therefore special, and are called canonical. If also

$$h(Q_i, P_i, t) = H(q_i(Q_i, P_i, t), p_i(Q_i, P_i, t), t),$$

where the Hamilton function satisfies the Hamilton equations in the coordinates q_i and p_i , it is called a proper canonical transformation, but this is not required for a transformation to be canonical. This is a very important distinction. Proper canonical transformations provide a constructive way to create the Hamilton function. Improper canonical transformations only require the existence of some Hamilton function such that (5.25-5.26) is fulfilled. No tool is yet provided to proof the existence of such a canonical transformation, lest alone construct it. Finding (im)proper canonical transformations could therefore be much more complicated.

To get a better idea of how far canonical transformation can go, it is best to consider first an example, before trying to construct general tests for canonicity of transformations.

As a first example, consider a transformation which exchanges generalized coordinates and momenta,

$$Q_i = -p_i \quad (5.27)$$

$$P_i = q_i. \quad (5.28)$$

This transformation is a proper canonical transformation, since for the Hamilton function $h(Q_i, -P_i, t) = H(-p_i, q_i, t)$

$$\begin{aligned} \frac{\partial h}{\partial P_i} &= \frac{\partial H}{\partial q_j} \frac{\partial q_j}{\partial P_i} = -d_t p_i = d_t Q_i \\ \frac{\partial h}{\partial Q_i} &= \frac{\partial H}{\partial p_j} \frac{\partial p_j}{\partial Q_i} = -d_t q_i = -d_t P_i. \end{aligned}$$

This is a quite remarkable result. It implies that generalized coordinates and momenta can be exchanged at will, or even partially. Hamilton's formulation does not distinguish between both, emphasizing again that the trajectory is the basic object, and the generalized coordinates and momenta are just description without inherent importance of their own.

So, how far can this be driven? Is it possible to find a canonical transformation which makes coordinates cyclic? Which makes all coordinates cyclic? Then, the problem

would become trivial. The answer to this is affirmative, and will be given in section 5.13. Unfortunately, while possible in principle, in practice this is often as hard as solving the original problem. But before this can be achieved, further developments are necessary. The first is finding a criterion for the canonicity of a transformation.

The first step is done by searching for a way how to construct for any canonical transformation the Hamilton function. To this end, two particular insights are important. First is that the trajectory should remain the same, though its parametrization may change. It therefore seems reasonable to give the generalized coordinates, though they are interchangeable with the generalized momenta, a special role. The second is the observation that the definition of the generalized momenta can be shifted by some arbitrary function of the coordinates, (5.22). Both together suggest to make the following ansatz,

$$p_i dq_i - H(p_i, q_i, t) = P_i dQ_i - h(P_i, Q_i, t) + d_t F_1(q_i, Q_i, t), \quad (5.29)$$

where the function F_1 is called the generator of the canonical transformation¹² between q_i and p_i , and Q_i and P_i . It will be shown that if this relation holds, then the transformation together with this new Hamilton function is a canonical transformation.

It is helpful to first show that if such a function exists, then it is unique. To do so, note that

$$d_t F_1 = \frac{\partial F_1}{\partial q_i} d_t q_i + \frac{\partial F_1}{\partial Q_i} d_t Q_i + \partial_t F_1. \quad (5.30)$$

As, with respect to F_1 , the variables q_i and Q_i are independent, the prefactors of $d_t q_i$ and $d_t Q_i$ must cancel with those of (5.29). This implies

$$\frac{\partial F_1}{\partial q_i} = p_i \quad (5.31)$$

$$\frac{\partial F_1}{\partial Q_i} = -P_i \quad (5.32)$$

$$\partial_t F_1(q_i(Q_i, P_i, t), Q_i, t) = h(Q_i, P_i, t) - H(q_i(Q_i, P_i, t), p_i(Q_i, P_i, t), t). \quad (5.33)$$

Thus, up to an irrelevant constant, F_1 is uniquely determined, as all derivatives are fixed by known quantities. Note that this still yields no constructive way of determining h and thus F_1 . Of course, if either F_1 or h are known, this will yield the other.

It still remains to show that the associated transformation is canonical. For this, Hamilton's principle will be used. Consider thus the action S of (5.1), but reexpress the Lagrange function by the Hamilton function. Replacing the original Hamilton function using (5.29) yields

$$S = \int_{t_1}^{t_2} dt (P_i d_t Q_i - h + d_t F_1) = \int_{t_1}^{t_2} dt (P_i d_t Q_i - h) + F_1|_{t_1}^{t_2} = s + F_1|_{t_1}^{t_2}.$$

¹²The meaning of the index 1 will become apparent later.

Performing the variation with respect to the new variables yields

$$\delta S = \delta s + \left. \frac{\partial F_1}{\partial Q_i} \delta Q_i \right|_{t_1}^{t_2} \quad (5.34)$$

There is now one important aspect to be taken into account. The point transformation (5.23-5.24) make the new variables Q_i dependent on the old canonical momenta. The boundary conditions on the path q_i required them to have fixed values at the times t_1 and t_2 . However, there has been no conditions for the generalized momenta. Therefore, the values of the Q_i at these times still depend on the generalized momenta at these times. Since the varied trajectories can have different canonical momenta at the initial and final times, the corresponding Q_i belonging to the original trajectories may change at the initial and final times, and the variations at the initial and final times of the Q_i can therefore potentially not vanish.

This subtlety can be taken care of by a partial integration

$$\delta S = \int_{t_1}^{t_2} dt \left((\delta P_i) d_t Q_i + P_i \delta d_t Q_i - \frac{\partial h}{\partial Q_i} \delta Q_i - \frac{\partial h}{\partial P_i} \delta P_i \right) + \left. \frac{\partial F_1}{\partial Q_i} \delta Q_i \right|_{t_1}^{t_2} \quad (5.35)$$

$$= \int_{t_1}^{t_2} dt \left(\left(d_t Q_i - \frac{\partial h}{\partial P_i} \right) \delta P_i - \left(d_t P_i + \frac{\partial h}{\partial Q_i} \right) \delta Q_i \right) + \left(P_i + \frac{\partial F_1}{\partial Q_i} \right) \delta Q_i \Big|_{t_1}^{t_2} \quad (5.36)$$

The relation (5.32) implies that the term involving F_1 vanishes. Since δS still needs to vanish, as it is only a rewriting of the the original Hamilton's principle in the old coordinates, this implies (5.25-5.26). But this is just the condition for the transformation to be canonical. Hence, given any arbitrary function F_1 , a canonical transformation is created. The new generalized coordinates and momenta Q_i and P_i are obtained by solving the equations (5.31) and (5.32) for them. This resolving of the equations may actually be involved. The new Hamilton operator is obtained from (5.33). This also implies that if F_1 does not depend explicitly on the time the canonical transformation is proper.

5.8 Alternative formulations of canonical transformations

As noted in the previous sections, generalized coordinates and momenta are exchangeable concepts. It therefore appears suspicious that the generating function for canonical transformations should depend particularly on the coordinates. On the other hand, it has been shown that the generating function is unique for a given transformation.

This discrepancy can be resolved by again separating the concepts cleanly. The transformation describes an invertible (and differentiable) map of the state space into itself. The function F_1 is a particular, coordinate-dependent representation of this map. The map itself is coordinate-independent. Therefore, it can be expressed in any sets of coordinates. Therefore, it must also be expressible in any set of coordinates.

To obtain the other three logical possibilities

$$F_2(q_i, P_i, t)$$

$$F_3(p_i, Q_i, t)$$

$$F_4(p_i, P_i, t),$$

it should be sufficient to reexpress the original function F_1 and the new Hamilton function h in those sets of coordinates. But the corresponding transformations are known due to the relations (5.31-5.33). However, as the differentials and invertibility of F_1 play important roles, the transformation cannot be done by merely replacing the arguments. Rather, they will again be obtained by a Legendre transformation, as described in section 5.3. It is not possible to obtain a generating function containing only the old or the new coordinates, as such a function would contain no information on the relation between both sets of variables. Note also that there is no general optimal choice which of the F_i are best suited. It depends on the problem at hand, which of them yields the most simple result. This will be exemplified in some examples after their equivalence has been established.

This will be exemplified in detail for one of the functions, F_2 , while for the others only the relevant results will be given. They are obtained in the same manner.

The function F_2 is obtained by a Legendre transformation (5.8) of F_1 on the variable Q_1 to P_1 . Thus,

$$F_2(q_i, P_i, t) = F_1(q_i, Q_i, t) - \frac{\partial F}{\partial Q_i} Q_i = F_1(q_i, Q_i(q_i, P_i, t), t) + P_i Q_i(q_i, P_i, t).$$

Note that F_2 is uniquely determined by F_1 , as has been discussed in section 5.3, and it is therefore not necessary to show that it is unique.

This implies for the relevant total temporal derivative, using (5.30),

$$d_t F_2 = \frac{\partial F_2}{\partial Q_i} d_t q_i + \frac{\partial F_2}{\partial P_i} d_t P_i + \partial_t F_2 = d_t F_1 + Q_i d_t P_i + P_i d_t Q_i = p_i d_t q_i + Q_i d_t P_i + h - H.$$

Comparing again term by term yields the relations

$$\frac{\partial F_2}{\partial q_i} = p_i \quad (5.37)$$

$$\frac{\partial F_2}{\partial P_i} = Q_i \quad (5.38)$$

$$\frac{\partial F_2}{\partial t} = h - H, \quad (5.39)$$

and thus a very similar form as (5.31-5.33).

To show that this also represents a canonical transformation, it is best to express the Lagrange function, following, (5.29), using F_2 ,

$$L = p_i d_t q_i - H = P_i d_t Q_i - h + d_t F_1 = P_i d_t Q_i - h + d_t F_2 - P_i d_t Q_i + Q_i d_t P_i = -Q_i d_t P_i - h + d_t F_2.$$

This result can be entered in the action, and using the same line of arguments as in (5.34-5.36), but using (5.37-5.39) instead of (5.31-5.33), yields again that the transformation is canonical, and proper canonical if it does not depend explicitly on time.

In exactly the same way the analogue of (5.31-5.33) are obtained for F_3 and F_4 , yielding

$$\begin{aligned} \frac{\partial F_3}{\partial p_i} &= -q_i \\ \frac{\partial F_3}{\partial Q_i} &= P_i \\ \frac{\partial F_3}{\partial t} &= h - H \\ \frac{\partial F_4}{\partial p_i} &= -q_i \\ \frac{\partial F_4}{\partial P_i} &= Q_i \\ \frac{\partial F_4}{\partial t} &= h - H. \end{aligned}$$

The occasionally appearing minus sign here and in (5.31-5.33) and (5.37-5.39) stem from those in (5.11-5.13). Their origin will be discussed in more detail in section 6.5. It is not surprising that the partial derivatives with respect to time are always the same. As they are deciding whether a canonical transformation is proper, they need to be the same, as being proper is a coordinate-independent statement.

After these more formal developments, it is useful to consider a few examples to show how these principles are applied.

The first is to formalize the transformation exchanging generalized momenta and coordinates using this framework. This is achieved by

$$F_1 = -q_i Q_i$$

since

$$\begin{aligned} p_i &= \frac{\partial F_1}{\partial q_i} = -Q_i \\ P_i &= -\frac{\partial F_1}{\partial Q_i} = q_i, \end{aligned}$$

in agreement with (5.27-5.28). It is also proper, as F_1 does not depend explicitly on time. To give an example of a reformulation, consider

$$F_4 = -p_i P_i,$$

which yields the same transformation. It can also be obtained as a double Legendre transformation of F_1 .

It is often useful to change the coordinate system of the generalized coordinates, i. e. $Q_i = f_i(q_j)$. This is also a proper canonical transformation, and generated by

$$\begin{aligned} F_2 &= f_i P_i \\ Q_i &= \frac{\partial F_2}{\partial P_i} = f_i \\ p_i &= \frac{\partial F_2}{\partial q_i} = \frac{\partial f_j}{\partial q_i} P_j. \end{aligned}$$

The last equation is a system of linear equations with a transformation matrix $A_{ij} = \partial f_i / \partial q_j$. Since a coordinate transformation must be invertible, this matrix is also invertible, yielding

$$P_i = (A^{-1})_{ij} p_j.$$

This implies that a change of coordinate system also changes the generalized momenta. The choice $f_i = q_i$ is then an identity transformation where the new and old coordinates coincide. The identity transformation is therefore also a canonical transformation¹³.

Finally, to demonstrate the value, at least in principle, of a canonical transformation, consider the harmonic oscillator with Hamilton function

$$H = \frac{p^2}{2m} + \frac{m\omega_0^2}{2} q^2,$$

where it does not matter whether this is indeed a harmonic oscillator or whether the problem in suitable generalized coordinates just takes the form of a harmonic oscillator.

Consider the generating function

$$\begin{aligned} F_1 &= \frac{m\omega_0 q^2}{2} \cot Q \\ p &= \frac{\partial F_1}{\partial q} = m\omega_0 q \cot Q \\ P &= -\frac{\partial F}{\partial Q} = \frac{m\omega_0^2 q^2}{2 \sin^2 Q}. \end{aligned}$$

¹³Incidentally, this shows that canonical transformation form a group: There is an identity, two canonical transformation are again a canonical transformation, there exists an inverse transformation, and the transformations are associative and closed.

Solving these equations for q and p yields

$$q = \sqrt{\frac{2P}{m\omega_0}} \sin Q \quad (5.40)$$

$$p = \sqrt{2m\omega_0 P} \cos Q. \quad (5.41)$$

Since the generating function does not depend on time the new Hamilton function is

$$H(q(Q, P), p(Q, P)) = P\omega_0 \cos^2 Q + \omega_0 P \sin^2 Q = \omega_0 P.$$

Thus, the coordinate Q is cyclic, and the solution is

$$\begin{aligned} P(t) &= P(0) \\ Q(t) &= \omega_0 t + Q_0. \end{aligned}$$

Reinserting this into (5.40-5.41) yields then the familiar solutions of the harmonic oscillator from section 2.6. Thus, the canonical transformation lead to trivializing the problem. Therefore, a good choice of a canonical transformation can substantially reduce the complexity of a given problem. This will be further developed in section 5.13.

Another interesting example is the transformation (4.17) of section 4.5. This transformation is obtained from the generating function

$$F_2(q_i, P_i, t) = q_i P_i - f(q_i, t)$$

where $f(q_i, t)$ is the same function as in (4.17). This yields

$$\begin{aligned} Q_i &= \frac{\partial F_2}{\partial P_i} = q_i \\ P_i &= \frac{\partial F_2}{\partial q_i} = P_i - \frac{\partial f}{\partial q_i} \\ h &= H + \partial_t F_2 = H - \partial_t f, \end{aligned}$$

and thus the same result as in section 4.5.

5.9 Poisson brackets

A transformation can be most directly be identified to be canonical using a new concept, the so-called Poisson brackets, which will be developed in the following. Though it is in the end a very compact way of expressing the conditions of canonicity, the Poisson brackets are again a concept with an importance which will only become fully unveiled in quantum physics. The Poisson brackets will also be very useful to formulate many results

in a very compact way, though it can be argued whether this can be considered to be an advantage.

While it is possible to just define the Poisson brackets and then show its usefulness, it is arguably better to show that it emerges automatically from a very general question. This question is: Given a classical mechanical system, there may be many quantities of interest. So far, the main focus were on the trajectories of the individual particles. However, other questions may be much more interesting. E. g., how often particles collide, how many particles appear in which area of the system, how often does a particle orbit another particle before escaping to infinity. This list can be extended arbitrarily and infinitely.

Since any mechanical system is uniquely characterized by a state, any such observable f can only depend on the state, i. e. the generalized coordinates, momenta, and the time, $f(p_i, q_i, t)$. An interesting question is, how this quantity changes with time. Of course, solving the system and inserting the results for the generalized coordinates and momenta would answer this question. But it is very often the case that it is already sufficient to know the answer as a function of the generalized quantities. Especially, this provides a result independent of any particular initial conditions, which are needed for any concrete realizations of the trajectories.

The answer to this question is

$$d_t f = \frac{\partial f}{\partial q_i} d_t q_i + \frac{\partial f}{\partial p_i} d_t p_i + \partial_t f = \frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} + \partial_t f, \quad (5.42)$$

where in the second step Hamilton's equations of motion (5.11-5.12) have been used.

This result motivates to define the Poisson brackets as the following prescription. Given two functions f and g depending on two set of variables p_i and q_i , the Poisson brackets with respect to the two sets of variables is defined as

$$\{f, g\}_{q,p} = \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial g}{\partial q_i} \frac{\partial f}{\partial p_i}.$$

The name brackets originates from the curly braces on the left-hand-side. The Poisson brackets are therefore a mathematical operation, akin to, say, multiplication. In the context of classical mechanics the index pair p, q is usually dropped, if the generalized coordinates and momenta are referred to, then writing $\{f, g\}$.

The result (5.42) can therefore be expressed using the Poisson bracket as

$$d_t f = \{f, H\} + \partial_t f. \quad (5.43)$$

Thus, up to any explicit time dependence, the time evolution of a mechanical quantity is determined by its Poisson bracket with the Hamilton function. This gives the Hamilton

function an extremely elevated conceptual importance, as it can therefore be considered as the source of evolution in time.

This is also emphasized by

$$\begin{aligned} d_t q_i &= \{q_i, H\} = \frac{\partial q_i}{\partial q_j} \frac{\partial H}{\partial p_j} - \frac{\partial H}{\partial q_j} \frac{\partial q_i}{\partial p_j} = \delta_{ij} \frac{\partial H}{\partial p_j} = \frac{H}{\partial p_i} \\ d_t p_i &= \{p_i, H\} = \frac{\partial p_i}{\partial q_j} \frac{\partial H}{\partial p_j} - \frac{\partial H}{\partial q_j} \frac{\partial p_i}{\partial p_j} = -\delta_{ij} \frac{\partial H}{\partial q_j} = -\frac{H}{\partial q_i}, \end{aligned}$$

giving a reformulation of Hamilton's equations (5.11-5.12) using the Poisson brackets. Therefore, Hamilton's equations can be considered as special cases of the more general time evolution equation (5.43).

A special case are also the so-called fundamental Poisson brackets

$$\{q_j, q_k\} = \frac{\partial q_j}{\partial q_i} \frac{\partial q_k}{\partial p_i} - \frac{\partial q_k}{\partial q_i} \frac{\partial q_j}{\partial p_i} = 0 \quad (5.44)$$

$$\{p_j, p_k\} = \frac{\partial p_j}{\partial q_i} \frac{\partial p_k}{\partial p_i} - \frac{\partial p_k}{\partial q_i} \frac{\partial p_j}{\partial p_i} = 0 \quad (5.45)$$

$$\{q_j, p_k\} = \frac{\partial q_j}{\partial q_i} \frac{\partial p_k}{\partial p_i} - \frac{\partial p_k}{\partial q_i} \frac{\partial q_j}{\partial p_i} = \delta_{ji} \delta_{ki} = \delta_{jk}. \quad (5.46)$$

These are the Poisson brackets of the sets of variables itself, therefore the name fundamental, as these are the most elementary Poisson brackets since no further function is involved. Thus, only mixed fundamental Poisson brackets do not vanish. Though these seem to be comparatively simple statements, modifications of the relations (5.44-5.46) can serve as the fundamental postulates of quantum physics.

The time evolution equation (5.43) has a particular interesting implication for constants of motions, i. e. for quantities with $d_t f = 0$. In this case

$$0 = d_t f = \{f, H\} + \partial_t f.$$

This criterion is often much easier to check than any other criteria, besides cyclic coordinates, found so far, as it does not require the explicit solution of the equations of motion. Especially, for any not explicitly time-dependent quantity it follows that

$$\{f(q_i, p_i), H\} = 0 \Rightarrow d_t f = 0, \quad (5.47)$$

and is a very compact test for conserved quantities. For the Hamilton function itself this implies

$$d_t H = \{H, H\} + \partial_t H = \partial_t H,$$

i. e. the statement of section 4.8.1 is recovered that the Hamilton function is conserved if it does not depend explicitly on time. This will be put in a different perspective in section 5.12 below.

5.10 Poisson brackets and (canonical) transformations

One of the most important features of the equations of motions, as discussed already for the Lagrange equations of the second kind in section 4.5, is that they do not depend on a particular coordinate system, and that they keep the same form in any coordinate system. Studying this feature in detail for the Poisson brackets, and thus especially of the dynamical time evolution formulated in (5.43), will lead back to the canonical transformations of section 5.7.

Consider two sets of generalized variables q_i and p_i , as well as Q_i and P_i , such that the relations

$$\begin{aligned} Q_i &= Q_i(p_j, q_j) \\ P_i &= P_i(p_j, q_j) \end{aligned}$$

are invertible relations, i. e. there are uniquely defined functions

$$\begin{aligned} q_i &= q_i(Q_j, P_j) \\ p_i &= p_i(Q_j, P_j), \end{aligned}$$

just as in section 4.5. In particular,

$$H(p_i, q_i) = H(q_i(Q_j, P_j), p_i(Q_k, P_k)) = H(Q_l, P_l),$$

i. e. the change of variables is canonical. Especially, just as in section 4.5, it can be shown that Hamilton's equations (5.11-5.13) hold in the same form in the new variables.

Consider

$$\begin{aligned} d_t Q_j &= \frac{\partial Q_j}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial H}{\partial q_i} \frac{\partial Q_j}{\partial p_i} = \frac{\partial Q_j}{\partial q_i} \left(\frac{\partial H}{\partial Q_k} \frac{\partial Q_k}{\partial p_i} + \frac{\partial H}{\partial P_k} \frac{\partial P_k}{\partial p_i} \right) - \frac{\partial Q_j}{\partial p_i} \left(\frac{\partial H}{\partial Q_k} \frac{\partial Q_k}{\partial q_i} + \frac{\partial H}{\partial P_k} \frac{\partial P_k}{\partial q_i} \right) \\ &= \frac{\partial H}{\partial Q_k} \left(\frac{\partial Q_j}{\partial q_i} \frac{\partial Q_k}{\partial p_i} - \frac{\partial Q_k}{\partial q_i} \frac{\partial Q_j}{\partial p_i} \right) + \frac{\partial H}{\partial P_k} \left(\frac{\partial Q_j}{\partial q_i} \frac{\partial P_k}{\partial p_i} - \frac{\partial P_k}{\partial q_i} \frac{\partial Q_j}{\partial p_i} \right) \\ &= \frac{\partial H}{\partial Q_k} \{Q_j, Q_k\} + \frac{\partial H}{\partial P_k} \{Q_j, P_k\}. \end{aligned}$$

Since the same set of Hamilton's equation must hold for the new variables, this implies

$$\{Q_i, Q_j\} = \{P_i, P_j\} = 0 \quad (5.48)$$

$$\{Q_i, P_j\} = \delta_{ij}. \quad (5.49)$$

The time evolution of P_j furthermore shows, in exactly the same way, $\{P_i, P_k\} = 0$.

Though this implies that the fundamental Poisson brackets have the same form, no matter the choice of coordinates, it still needs to be answered what happens in the general case. In a similar fashion as before it follows that

$$\begin{aligned}
 \{f, g\} &= \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial g}{\partial q_i} \frac{\partial f}{\partial p_i} = \frac{\partial f}{\partial q_i} \left(\frac{\partial g}{\partial Q_j} \frac{\partial Q_j}{\partial p_i} + \frac{\partial g}{\partial P_j} \frac{\partial P_j}{\partial p_i} \right) - \frac{\partial f}{\partial p_i} \left(\frac{\partial g}{\partial Q_j} \frac{\partial Q_j}{\partial q_i} + \frac{\partial g}{\partial P_j} \frac{\partial P_j}{\partial q_i} \right) \\
 &= \frac{\partial g}{\partial Q_l} \left(\frac{\partial f}{\partial q_i} \frac{\partial Q_l}{\partial p_i} - \frac{\partial Q_l}{\partial q_i} \frac{\partial f}{\partial p_i} \right) + \frac{\partial g}{\partial P_l} \left(\frac{\partial f}{\partial q_i} \frac{\partial P_l}{\partial p_i} - \frac{\partial P_l}{\partial q_i} \frac{\partial f}{\partial p_i} \right) \\
 &= \frac{\partial g}{\partial Q_l} \{f, Q_l\} + \frac{\partial g}{\partial P_l} \{f, P_l\}.
 \end{aligned}$$

Before continuing, it is useful to note two particular cases of this result for future use, when setting f either to the new generalized coordinates or momentum,

$$\begin{aligned}
 \{g, Q_i\} &= -\frac{\partial g}{\partial P_i} \\
 \{g, P_i\} &= \frac{\partial g}{\partial Q_i},
 \end{aligned}$$

where it should be kept in mind that, in line with the conventions, the Poisson brackets are still evaluated with respect to the generalized quantities p_j and q_j .

These two results can be used also in the original expression, yielding

$$\{f, g\}_{q,p} = \frac{\partial g}{\partial Q_i} \left(-\frac{\partial f}{\partial P_i} \right) + \frac{\partial g}{\partial P_i} \frac{\partial f}{\partial Q_i} = \{f, g\}_{Q,P},$$

i. e. also the Poisson brackets remain form-invariant under a change of variables. In particular, the dynamical equation (5.43) takes the same form in any system of generalized quantities.

This feature can now be used to check if a given variable transformation is canonical. To prepare this, it is useful to consider first a check using the generating functionals.

Consider some new variables Q_i and P_i . If they are obtained from a canonical transformation, there must exist also the corresponding generating functions F_i . Given, e. g., F_1 , canonicity would imply

$$\begin{aligned}
 p_i &= \frac{\partial F_1}{\partial q_i} \\
 P_i &= -\frac{\partial F_2}{\partial Q_i}.
 \end{aligned}$$

Differentiating both equations once more with respect to any of the other variables leads

to

$$\left. \frac{\partial p_i}{\partial Q_j} \right|_{t,q,Q_k \neq j} = \frac{\partial^2 F_1}{\partial Q_j \partial q_i} = \frac{\partial^2 F_1}{\partial q_i \partial Q_j} = \left. \frac{\partial P_j}{\partial q_i} \right|_{t,Q,q_k \neq i} \quad (5.50)$$

$$\left. \frac{\partial p_i}{\partial q_j} \right|_{t,Q,q_k \neq j} = \left. \frac{\partial P_j}{\partial q_i} \right|_{t,Q,q_k \neq i} \quad (5.51)$$

$$\left. \frac{\partial p_i}{\partial Q_j} \right|_{t,q,Q_k \neq j} = \left. \frac{\partial P_j}{\partial Q_i} \right|_{t,q,Q_k \neq i}. \quad (5.52)$$

Similar expressions can be obtained from any of the other F_i s, just that the derivatives are then with respect to other variables. At any rate, the result implies that certain derivatives of the new and old variables have to coincide. In fact, all of the relations have to be fulfilled. The fact that second derivatives of the generating functions have to coincide is actually conceptually significant, as it already hints at a certain structure, as discussed in section 6.5, though this partially enters regions of function theory not yet available.

However, in practical calculations this test is rather unwieldy. Using Poisson brackets, it is possible to reformulate it in much more convenient ways. The following will be done for proper canonical transformation for simplicity. An extension to general canonical transformation is possible, but tedious. Rather, it will be shown that if (5.48-5.49) hold, then the transformation is canonical. So far it has also been show that if the transformation is canonical they hold. Thus, the next step is to prove the reverse, and make it an equivalence.

Since it does not matter which variables are used, see section 5.8, only one possibility will be investigated here. Irrespective of whether a transformation is canonical or not, it is always possible to evaluate the Poisson brackets for the new variables in terms of the old ones. Also, for any quantity (5.43) holds. Thus,

$$\begin{aligned} \partial_t Q_i &= \{Q_i, H\} = \frac{\partial Q_i}{\partial q_j} \frac{\partial H}{\partial p_j} - \frac{\partial Q_i}{\partial p_j} \frac{\partial H}{\partial q_j} \\ &= \frac{\partial Q_i}{\partial q_j} \left(\frac{\partial h}{\partial Q_k} \frac{\partial Q_k}{\partial p_j} + \frac{\partial h}{\partial P_k} \frac{\partial P_k}{\partial p_j} \right) - \frac{\partial Q_i}{\partial p_j} \left(\frac{\partial h}{\partial Q_k} \frac{\partial Q_k}{\partial q_j} + \frac{\partial h}{\partial P_k} \frac{\partial P_k}{\partial q_j} \right) \\ &= \frac{\partial h}{\partial Q_k} \{Q_i, Q_k\} + \frac{\partial h}{\partial P_k} \{Q_i, P_k\}. \end{aligned}$$

Completely analogous follows

$$\partial_t P_i = -\frac{\partial h}{\partial Q_k} \{Q_k, P_i\} + \frac{\partial h}{\partial P_k} \{P_i, P_k\}.$$

Both results together imply that the transformation is (proper) canonical, and thus that Hamilton's equations take the same form also in the new coordinates, if and only if (5.48-5.49) hold. This completes the proof, and implies that also generating functions exist. However, the proof is not constructive, and does not yield them.

5.11 The Poisson bracket as a differential operator

The Poisson brackets can be used to establish a more abstract mathematical framework in mechanics, which will be pursued further in section 6.5. Before laying the foundations for it, it is useful to collect a few properties of the Poisson brackets.

First of all, the results (5.44-5.45) are special cases of the more general statements

$$\begin{aligned}\{f, f\} &= \frac{\partial f}{\partial q_i} \frac{\partial f}{\partial p_i} - \frac{\partial f}{\partial q_i} \frac{\partial f}{\partial p_i} = 0 \\ \{f(q_j), g(q_k)\} &= \frac{\partial f(q_j)}{\partial q_i} \frac{\partial g(q_k)}{\partial p_i} - \frac{\partial g(q_k)}{\partial q_i} \frac{\partial f(q_j)}{\partial p_i} = 0 \\ \{f(p_j), g(p_k)\} &= \frac{\partial f(p_j)}{\partial q_i} \frac{\partial g(p_k)}{\partial p_i} - \frac{\partial g(p_k)}{\partial q_i} \frac{\partial f(p_j)}{\partial p_i} = 0\end{aligned}\tag{5.53}$$

which hold true for any sufficiently often continuously differentiable functions. It is thus (5.46) which holds the non-trivial information. The Poisson brackets also vanish if either or both of the arguments are constant,

$$\{c, g(p_j, q_j)\} = \frac{\partial c}{\partial q_i} \frac{\partial g(p_j, q_j)}{\partial p_i} - \frac{\partial g(p_j, q_j)}{\partial q_i} \frac{\partial c}{\partial p_i} = 0.\tag{5.54}$$

They therefore act non-trivially only on functions.

The Poisson brackets are antisymmetric under the exchange of its arguments

$$\{f, g\} = \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial g}{\partial q_i} \frac{\partial f}{\partial p_i} = - \left(\frac{\partial g}{\partial q_i} \frac{\partial f}{\partial p_i} - \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} \right) = -\{g, f\}.\tag{5.55}$$

From this (5.53) follows immediately without calculation.

The Poisson brackets are a linear operation for any function f_i and constants c_i ,

$$\begin{aligned}\{c_1 f_1 + c_2 f_2, f_3\} &= \frac{\partial(c_1 f_1 + c_2 f_2)}{\partial q_i} \frac{\partial f_3}{\partial p_i} - \frac{\partial f_3}{\partial q_i} \frac{\partial(c_1 f_1 + c_2 f_2)}{\partial p_i} \\ &= c_1 \left(\frac{\partial f_1}{\partial q_i} \frac{\partial f_3}{\partial p_i} - \frac{\partial f_3}{\partial q_i} \frac{\partial f_1}{\partial p_i} \right) + c_2 \left(\frac{\partial f_2}{\partial q_i} \frac{\partial f_3}{\partial p_i} - \frac{\partial f_3}{\partial q_i} \frac{\partial f_2}{\partial p_i} \right) \\ &= c_1 \{f_1, f_3\} + c_2 \{f_2, f_3\},\end{aligned}\tag{5.56}$$

and products expand like

$$\begin{aligned}\{f_1 f_2, f_3\} &= \frac{\partial(f_1 f_2)}{\partial q_i} \frac{\partial f_3}{\partial p_i} - \frac{\partial f_3}{\partial q_i} \frac{\partial(f_1 f_2)}{\partial p_i} \\ &= f_1 \left(\frac{\partial f_2}{\partial q_i} \frac{\partial f_3}{\partial p_i} - \frac{\partial f_3}{\partial q_i} \frac{\partial f_2}{\partial p_i} \right) + \left(\frac{\partial f_1}{\partial q_i} \frac{\partial f_3}{\partial p_i} - \frac{\partial f_3}{\partial q_i} \frac{\partial f_1}{\partial p_i} \right) f_2 \\ &= f_1 \{f_2, f_3\} + \{f_1, f_3\} f_2,\end{aligned}\tag{5.57}$$

and likewise for other expressions by usage of the antisymmetry (5.55). Note also that, for x any variable,

$$\partial_x \{f, g\} = \partial_x \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial g}{\partial q_i} \frac{\partial f}{\partial p_i} \right) = \{\partial_x f, g\} + \{f, \partial_x g\}, \quad (5.58)$$

and thus the product rule for ordinary differentials applies also to Poisson brackets.

It is possible to create double Poisson brackets,

$$\begin{aligned} \{f, \{g, h\}\} &= \left\{ f, \frac{\partial g}{\partial q_i} \frac{\partial h}{\partial p_i} - \frac{\partial h}{\partial q_i} \frac{\partial g}{\partial p_i} \right\} \\ &= \frac{\partial f}{\partial q_j} \frac{\partial}{\partial p_j} \left(\frac{\partial g}{\partial q_i} \frac{\partial h}{\partial p_i} - \frac{\partial h}{\partial q_i} \frac{\partial g}{\partial p_i} \right) - \frac{\partial f}{\partial p_j} \frac{\partial}{\partial q_j} \left(\frac{\partial g}{\partial q_i} \frac{\partial h}{\partial p_i} - \frac{\partial h}{\partial q_i} \frac{\partial g}{\partial p_i} \right), \end{aligned}$$

creating in total eight terms, each term having one second derivative and two first derivatives. Explicitly performing such calculations, it is possible to show that

$$\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0, \quad (5.59)$$

which is known as the Jacobi identity.

The Poisson brackets have thus a number of features familiar from differential operators: They yield zero when acting on a constant, (5.54), are linear operators, (5.56), and obey a product rule, (5.57). They are therefore considered to be a differential operator, expressed as

$$\{f, g\} = D_f g,$$

where the differential operator is D_f , sometimes also written as

$$D_f = \{f, \cdot\}.$$

In contrast to an ordinary differential operator it is a parametrized differential operator, as it depends on the function f . Such generalizations of differential operators play an important part of formal theory developments.

In fact, the Poisson bracket is just one example, and serves here as a prototype, of a whole class of mathematical operations, which all satisfy the properties (5.53-5.59). Just to give another example, the so-called commutator of two square matrices A and B is defined as

$$[A, B] = AB - BA$$

also satisfies the same conditions, where the concept of a constant is taken by the unit matrix. These, and other generalizations, appear throughout physics, and especially in quantum physics.

To show the usefulness of the derived relations for the Poisson brackets consider the following question: Given two conserved quantities, f and g , is it possible to find a non-trivial further conserved quantity from it? In fact, due to the Jacobi identity (5.59)

$$0 = \{f, \{g, H\}\} + \{g, \{H, f\}\} + \{H, \{f, g\}\} = \{\partial_t g, f\} + \{g, \partial_t f\} + \{H, \{f, g\}\}$$

it follows that

$$\{\{f, g\}, H\} + \partial_t \{f, g\} = 0.$$

Thus, the Poisson bracket of any two conserved quantities is again a conserved quantity. Of course, it is not possible to generate with this infinitely many non-trivial conserved quantities. At some point the Poisson brackets will give again just combinations of known conserved quantities. But often enough it is helpful for a construction of additional conserved quantities.

5.12 Poisson brackets and symmetries

Poisson brackets give another conceptual view on invariances and symmetries, and thus the conservation laws of section 4.8.

Consider an infinitesimal transformation of the coordinates and momenta

$$\begin{aligned} Q_i &= q_i + \delta q_i \\ P_i &= p_i + \delta p_i, \end{aligned}$$

where δx should for now only indicate that the quantity δx is small, and is not connected to displacements. If this is the case, the generating function needs to be only a small deviation from the identity transformation as well, e. g.

$$F_2 = q_i P_i + \epsilon G(q_i, P_i)$$

where G is some function and ϵ an infinitesimal parameter, small enough to make ϵG infinitesimal as well. Because of (5.37-5.38) it follows that

$$\begin{aligned} P_i - p_i &= \delta p_i = -\epsilon \frac{\partial G}{\partial q_i} \\ Q_i - q_i &= \delta q_i = \epsilon \frac{\partial G}{\partial P_i} \approx \epsilon \frac{\partial}{\partial P_i} \left(G(q_i, p_i) + \frac{\partial G(q_i, P_i)}{\partial P_i} \Big|_{P_i=p_i} (P_i - p_i) \right) = \epsilon \frac{\partial G(q_i, p_i)}{\partial p_i} \end{aligned}$$

where the last approximation is good, as a small change multiplied by ϵ is already smaller than ϵ .

So far, this is general. It is interesting to consider the case that $G = H$ and $\epsilon = dt$ a small interval in time. This leads to

$$\begin{aligned}\delta q_i &= dt \frac{\partial H}{\partial p_i} = \frac{dq_i}{dt} dt = dq_i \\ \delta p_i &= -dt \frac{\partial H}{\partial q_i} = \frac{dp_i}{dt} dt = dp_i.\end{aligned}$$

Thus, this canonical transformation actually pushes the generalized coordinates and momenta forward in time. This implies time evolution is equivalent to an (infinitesimal) canonical transformation. By consecutive such infinitesimal transformations ultimately the whole time evolution can be build. It is therefore valid to say that the Hamilton function creates the evolution in time, which is quite similar to the statement (5.43).

Consider now some arbitrary function of u , which changes as

$$\begin{aligned}\delta u &= u(q_i + \delta q_i, p_i + \delta p_i) - u(q_i, p_i) \\ &= \left(u(q_i, p_i) + \frac{\partial u}{\partial q_i} \delta q_i + \frac{\partial u}{\partial p_i} \delta p_i + \mathcal{O}(\delta q_i^2, \delta p_i^2, \delta q_i \delta p_i) \right) - u(q_i, p_i) \\ &\approx \frac{\partial u}{\partial q_i} \delta q_i + \frac{\partial u}{\partial p_i} \delta p_i \\ &= \epsilon \left(\frac{\partial u}{\partial q_i} \frac{\partial G}{\partial p_i} - \frac{\partial u}{\partial p_i} \frac{\partial G}{\partial q_i} \right) \\ &= \epsilon \{u, G\},\end{aligned}\tag{5.60}$$

where in the second line a Taylor expansion was performed. Thus, the change of a quantity u under some (infinitesimal) coordinate transformation G is determined by the Poisson bracket of this quantity with the coordinate transformation. Especially,

$$\delta H = \epsilon \{H, G\},\tag{5.61}$$

and thus also the Hamilton function itself changes in general.

If the function G is a constant of motion then, because of (5.47), its Poisson bracket with the Hamilton functions vanishes. In the present context, this implies that any coordinate transformation generated by an integral of motion leaves the Hamilton function unchanged.

This statement is actually a very deep one. As has been discussed in section 4.8 an integral of motion is usually associated with some symmetry of the Hamilton function. Thus, (5.60) together with (5.61) states that the integral of motions associated with a symmetry generate changes of quantities, but leave the Hamilton functions invariant. In fact, the function G will be seen to generate the transformation of any quantity under the corresponding symmetry transformation. In quantum physics, this will be the key to identify symmetries of the systems and the all the dynamical features of the theories. It is one of the key properties in the connection of symmetries and physics.

However, a full general proof of the connection is beyond the present scope. It will thus need to be sufficient to do so for some examples.

First consider that some coordinate j is cyclic and the transformation

$$\begin{aligned}\delta q_i &= \epsilon \delta_{ij} \\ \delta p_i &= 0.\end{aligned}\tag{5.62}$$

which requires $G = p_j$. Since H does not depend on p_j , this implies $\{H, G\} = 0$, realizing the aforementioned statement. The corresponding symmetry transformation is, according to (5.62), an infinitesimal translation in q_j , as this is the transformation performed. Thus, the integral of motion is connected with invariance, or translation symmetry, in the corresponding coordinate. Furthermore, the generator of this transformation is the conserved quantity.

As a second example consider Cartesian coordinates and a rotation around the z -axis. The corresponding change is

$$\begin{aligned}\delta x_i &= -y_i \delta \theta \\ \delta y_i &= x_i \delta \theta \\ \delta z_i &= 0.\end{aligned}$$

These changes are created by

$$G = x_i p_i^y - y_i p_i^x,$$

provided $\epsilon = \delta \theta$ is identified. G is then $G = L_z$, the z component of the total angular momentum. Again, if G is an integral of motion, because the system has symmetry around the z -axis as investigated in section 4.8, this function will have vanishing Poisson brackets with the Hamilton function.

On the other hand, note

$$\epsilon \{x_i, G\} = \delta \theta \left(\frac{\partial x_i}{\partial x_j} \frac{\partial G}{\partial p_j^x} - \frac{\partial G}{\partial x_j} \frac{\partial x_i}{\partial p_j^x} + (x \rightarrow y, z) \right) = -\delta \theta y_i,$$

and likewise for y_i or the momentum. Thus, indeed the Poisson bracket with the function G generates the transformation, in this case the rotation.

It is also very interesting to consider what happens for $u = L_x$. For simplicity, reduce this to a single particle. This yields

$$\begin{aligned}\{L_x, L_z\} &= \{yp_z - zp_y, xp_y - yp_x\} \\ &= \frac{\partial(yp_z - zp_y)}{\partial x_i} \frac{\partial(xp_y - yp_x)}{\partial p_i} - \frac{\partial(yp_z - zp_y)}{\partial p_i} \frac{\partial(xp_y - yp_x)}{\partial x_i} = -(zp_x - xp_z) = -L_y.\end{aligned}$$

Generalizing by permutation, this yields

$$\{L_i, L_j\} = \epsilon_{ijk} L_k.$$

Using (5.57) it also follows that

$$\{L^2, L_i\} = 2L_j\{L_j, L_i\} = 2\epsilon_{ijk} L_j L_k = 0.$$

These results hold in general. However, the conservation is only true if the system has rotational symmetry, and only then the components of the angular momentum generate rotations.

Note that the quantum versions of these expressions will play a very central role in quantum physics.

An interesting consequence can be obtained from these insights. As has been shown, the time-evolution along any trajectory in phase space is generated by the Hamilton function. Since trajectories are continuous functions, this is equivalent to an infinitesimal rotation and translation in phase space. Also, as noted in section 5.2, trajectories in phase space do not cross. This implies that a volume in phase space is surrounded by a dense set of trajectories as a surface. If no explicit time-dependence exist, this surface will not open when evolving in time, and trajectories on the inside cannot move outside, and vice versa. However, the shape of the surface, and thus of the volume, may change. As a consequence, the density of trajectories needs to remain constant over time. This is known as Liouville's theorem, and it will play an important role in statistical mechanics.

Note that similar considerations do not apply to either position space or configuration space. Thus, phase space, with its symplectic geometry, is the fundamental space of (classical) mechanics.

5.13 Hamilton-Jacobi theory

It will now be shown that it is possible to find for any mechanical problem, which is formulated by a Hamilton function, there exists a canonical transformation such that the problem becomes trivial. Trivial in this case means that it is either transformed to a known problem, or to a situation in which all coordinates become cyclic and the Hamilton function is explicitly time-independent or finally such that all generalized coordinates become constant, and thus yielding trivial Hamilton's equations.

The drawback is that, while this is possible in principle, it is often as complicated or more complicated than the original problem. The advantage is that, even if practically tedious, the knowledge that it is possible in principle helps often substantially in gaining conceptual insights. Thus, it is an important development.

5.13.1 General strategy

Explicit time-dependence of the Hamilton function plays an important role in which possibility of the three enumerated ones can be achieved. The second option cannot always be reached if there is explicit time-dependence, while the first one is often actually more involved, since it is often most easily achieved by first transforming to either of the second or third option and then back to the first one. Thus, the third option is the most attractive one, and will be the starting point.

The generalized coordinates will only be time-independent, if the Hamilton function is constant. This is necessarily the case if it is possible to find a canonical transformation such that

$$h = H + \partial_t F = 0,$$

as then all (partial) derivatives of the new Hamilton function vanish identically.

The following becomes most simple when searching for a generating function of type F_2 , though it is, of course, possible using any of the F_i . In this context, for reasons to become clear at the end of the derivation, F_2 is also called Hamilton's action function S .

This yields the Hamilton-Jacobi equation

$$H\left(q_i, \frac{\partial F_2}{\partial q_i}, t\right) + \partial_t F_2 = 0.$$

This is an implicit, in general non-linear as the generalized momenta enter quadratically, differential equation for F_2 . However, it is of at most first order in the variables of F_2 . Unfortunately, in contrast to ordinary differential equations, the mathematical theory of partial differential equations is much more involved, and it will require substantially more work to find a solution¹⁴. However, this implies that there will be as many initial conditions as derivatives, thus the number of generalized coordinates plus one for the time derivative. Given N generalized coordinates, this implies $N + 1$ integration constants. One is used up for the additive and irrelevant constant, leaving N .

As usual, the solution for F_2 is only unique up to a constant, since for any canonical transformation only the derivatives matter. Furthermore, in the equation only the derivatives of F_2 with respect to the momenta q_i enter, but not with respect to the P_i . This freedom will be used to identify the new generalized momenta with the N initial conditions. This ambiguity is due to the fact that point transformations of the generalized momenta are always a possible canonical transformation.

This yields the following strategy to create a trivial solution:

¹⁴Whether a solution for partial differential equations exist is in general a much more involved problem than for ordinary differential equations. But for any problem relevant in (conservative) mechanics the existence of such a solution can be taken to be guaranteed.

- (1) Write down the Hamilton-Jacobi differential equation
- (2) Find the solution F_2 - this is the tricky part. This yields $F_2(q_i, \alpha_i, t)$, where the α_i are the initial conditions. Since this does not constrain the dependence of F_2 on the α_i , it is admissible to identify in the following the α_i with the P_i

- (3) Solve

$$Q_i = \frac{\partial F_2}{\partial \alpha_i} = \beta_i.$$

Since F_2 satisfies the Hamilton-Jacobi equations, by definition the Q_i have to be constant. Then solve for the generalized coordinates q_i . This may again not be possible analytically in general. In principle, this is possible for any canonical transformations, yielding the generalized coordinates q_i as a function of the α_i , β_i and time only

- (4) Solve

$$p_i = \frac{\partial F_2}{\partial q_i}$$

to obtain the p_i as a function of the α_i , β_i and t . Again, this may not be possible analytically, but is possible in general

- (5) Determine the constants α_i and β_i from the initial conditions for the q_i and p_i . This then gives the q_i and p_i as a function of the initial conditions and the time, solving the problem

While this procedure guarantees a result the step 2, but also the steps 3-5, may in general only be possible numerically. In the next subsection, some examples in which it is possible analytically will be discussed.

5.13.2 A solution strategy

To outline the Hamilton-Jacobi strategy it is useful to consider the standard example of the harmonic oscillator with the Hamilton function

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2}q^2.$$

The Hamilton-Jacobi equations then takes the form

$$\frac{1}{2m} \left(\frac{\partial F_2}{\partial q} \right)^2 + \frac{m\omega^2}{2}q^2 + \partial_t F_2 = 0.$$

There is, even for this comparatively simple, case no obvious solution.

Based on experience, a good starting point is a so-called separation ansatz

$$F_2 = W(q) + V(t),$$

that is it is assumed that the dependence on the coordinates and on the time are additive¹⁵.

This yields

$$\frac{1}{2m} \left(\frac{dW}{dq} \right)^2 + \frac{m\omega^2}{2} q^2 = -d_t V.$$

Since the left-hand side does not depend on time and the right-hand side does not depend on q , this equation can only hold if both sides are equal to some constant γ .

The ensuing ordinary differential equation for V

$$\partial_t V = -\gamma$$

is solved by direct integration

$$V(t) = -\gamma t + V(0),$$

with initial condition $V(0)$.

Likewise, the ordinary differential equation

$$\frac{dW}{dq} = \sqrt{m^2\omega^2 \left(\frac{2\gamma}{m\omega^2} - q^2 \right)} \quad (5.63)$$

can also be solved by a (non-trivial) direct integration, yielding

$$W(q) = m\omega \left(\frac{q}{2} \sqrt{\frac{2\gamma}{m\omega^2} - q^2} + \frac{\gamma}{m\omega^2} \sin^{-1} \left(\sqrt{\frac{m\omega^2}{2|\gamma|}} q \right) \right) + W(0).$$

This yields the total function F_2

$$F_2 = m\omega \left(\frac{q}{2} \sqrt{\frac{2\gamma}{m\omega^2} - q^2} + \frac{\gamma}{m\omega^2} \sin^{-1} \left(\sqrt{\frac{m\omega^2}{2|\gamma|}} q \right) \right) - \gamma t + V(0) + W(0).$$

The sum $V(0) + W(0)$ is actually only a single independent integration constant, due to the separation ansatz. It is the constant shift of F_2 , as discussed in the previous subsection, and therefore plays no role in the following and can be set to zero. This leaves the new constant γ , which has to be identified with the second integration constant, $\gamma = \alpha$, required to solve the Hamilton-Jacobi equation. As required by the solution strategy, it is identified with the generalized momentum P .

¹⁵It is possible to worry whether making this ansatz excludes possible solutions. However, for partial differential equations of this type, so-called parabolic partial differential equations with no mixed terms, it can be shown that this is not the case.

The next step is to solve

$$Q = \frac{\partial F_2}{\partial \alpha} = \beta$$

This is actually simpler by first deriving (5.63) with respect to α and then to integrate with respect to q , yielding

$$\beta = \frac{\partial}{\partial \alpha} \int dq \frac{\partial F_2}{\partial q} = \int dq \frac{\partial^2 W}{\partial q \partial \alpha} - t = \frac{1}{\omega} \int dq \frac{1}{\omega \sqrt{\frac{2\alpha}{m\omega^2} - q^2}} = \frac{1}{\omega} \sin^{-1} \left(\sqrt{\frac{m\omega^2}{2\alpha}} q \right) - t.$$

This can be solved straightforwardly for q yielding

$$q = \sqrt{\frac{2\alpha}{m\omega^2}} \sin(\omega(t + \beta)),$$

which already has the form of the final solution, up to α and β , which still need to be determined by the initial conditions.

The generalized momentum is obtained by

$$q = \frac{\partial F_2}{\partial q} = \frac{dW}{dq} = m\omega \sqrt{\frac{2\alpha}{m\omega^2} - q^2} = \sqrt{2\alpha m} \cos(\omega(t + \beta)),$$

where the last step follows from a trigonometrical identity.

Finally, this requires to solve for α and β for the initial conditions. Choosing $q(0) = q_0$ and $p(0) = 0$ yields

$$\begin{aligned} \alpha &= \frac{m\omega^2 q_0^2}{2} = E \\ \beta &= \frac{\pi}{2\omega}, \end{aligned}$$

in which E is the total energy. The final step is to insert this into the solutions of q and p , yielding

$$\begin{aligned} q(t) &= \sqrt{\frac{2E}{m\omega^2}} \cos(\omega t) \\ p(t) &= -\sqrt{2Em} \sin(\omega t), \end{aligned}$$

as in section 2.6.

This result has also an interesting implication. The value of α is just the total energy, while β has dimension of time. Thus, the new canonical variables are energy and (a constant) time. Thus, energy and time are canonical conjugate variables. Though this is not necessarily the result of the Hamilton-Jacobi strategy, the fact that energy and time are canonical conjugate variables holds actually for quite a variety of systems.

The ansatz of a separation of variables made the solution of the problem in the previous subsection possible. As this type of ansatz is of great value far beyond the realm of mechanics, it is worthwhile to understand it better.

The actual reason why this approach worked out rather well was the fact that the time-dependence could be separated, because the Hamilton function did not depend on the time explicitly. In general, assume that $\partial_t H = 0$. The Hamilton-Jacobi equation takes then the form

$$H\left(q_i, \frac{\partial F_2}{\partial q_j}\right) + \partial_t F_2 = 0.$$

Again, the only case a time-derivative appears is in the second term. Make the ansatz

$$F_2 = W(q_i) - Et,$$

with E for now some constant. In the case of skleronom constraints E will usually turn out to be the total energy. This removes the time dependence from the Hamilton-Jacobi equation and yields

$$H\left(q_i, \frac{\partial W}{\partial q_j}\right) = E.$$

In this context W is called Hamilton's characteristic function. Note the constant E will in general depend on all the initial conditions still required to solve the equation for W . This implies that the canonical transformation satisfies

$$\begin{aligned} Q_i &= \frac{\partial W}{\partial \alpha_i} - \frac{\partial E}{\partial \alpha_i} t \\ p_i &= \frac{\partial W}{\partial q_i}, \end{aligned}$$

where the α_i are again the initial conditions for the Hamilton-Jacobi equation. This emphasizes that E , although being a constant, is not an inert quantity, but plays an important role in the final solution.

From here on the next steps are as before. The only difference is that the Hamilton-Jacobi equation for W has one variable less. This may seem like not a big gain, but in practice this is often a fundamental advantage¹⁶. Considering special relativity, this is actually less surprising. Time plays a quite different role than space, the latter being Euclidean. By reducing to a spatial problem, many things simplify. Of course, this may not be true for generalized coordinates, but often it is still so.

This procedure can be continued, if one of the variables, say q_1 , only appears as

$$H\left(q_{i \neq 1}, \frac{\partial W}{\partial q_{i \neq 1}}, f_1\left(q_1, \frac{\partial W}{\partial q_1}\right)\right) - E = 0.$$

¹⁶This will become even more apparent once treating the quantum-mechanical version of the problem.

Just as before, since all variables are independent, the ansatz

$$W(q_i) = W'(q_{i \neq 1}) + W_1(q_1)$$

with

$$\begin{aligned} f_1 \left(q_1, \frac{dW_1}{dq_1} \right) &= c_1 \\ H \left(q_{i \neq 1}, \frac{\partial W}{\partial q_{i \neq 1}}, c_1 \right) - E &= 0 \end{aligned}$$

is possible. Thus, the equation for W_1 becomes an ordinary differential equation, with the solution involving one of the integration constants. At the same time, c_1 , just as E , depends on all the integration constants. This reduces the complexity further, as an ordinary differential equation is much simpler to solve, and one variable less in a partial differential equation is also often a substantial simplification. Of course, if also for some of the other variables such a structure emerges, this procedure can be repeated. In the ideal case, the problem can be entirely reduced in this way, and is therefore equivalent to a set of ordinary differential equations. If this is the case, the Hamilton-Jacobi equation is said to be separable.

If all but one generalized coordinate are cyclic, the Hamilton-Jacobi equation is, almost by definition, separable, as the Hamilton-Jacobi equation itself is then already an ordinary differential equation. In this case, a suitable ansatz is

$$W = W_1(q_1) + \sum_{i \neq 1} \alpha_i q_i,$$

which induces the identity transformation of section 5.8 for all but the one non-cyclic variable. The constants α_i will then take the role of the new generalized momenta and integration constants. If only the generalized constants starting from some k should be cyclic, this implies that in this case

$$W = W'(q_1, \dots, q_{k-1}) + \sum_{i \geq k} \alpha_i q_i$$

is a suitable ansatz, and this will maintain the cyclicity of those generalized coordinates which are already cyclic.

Whether the Hamilton-Jacobi equation is separable or not is actually not a question of the system, but merely of the choice of variables. Evidently, since any mechanical system can, at least in principle, be reduced to a constant Hamilton function by usage of the Hamilton-Jacobi strategy, this final form of the problem is always separable: Since the

Hamilton function is constant and does not depend on any of the variables, the functions f_i are all trivial. This emphasizes again how important a good choice of generalized coordinates is¹⁷.

It is useful to investigate a few more examples with this strategy, due to the importance of it far beyond mechanics.

Consider the central potential problem of section 2.7. Its Hamilton function is

$$H = \frac{1}{2m} \left(p_r^2 + \frac{p_\phi^2}{r^2} \right) + V(r),$$

where it has already been used that angular momentum conservation enforces a movement in the plane with the radius variable r and the angle ϕ together with their respective generalized momenta. Since ϕ is cyclic, the problem is separable, and the ansatz for W is

$$W = W_1(r) + \alpha_\phi \phi.$$

This yields the Hamilton-Jacobi equation

$$\frac{1}{2m} \left(\left(\frac{\partial W}{\partial r} \right)^2 + \frac{1}{r^2} \left(\frac{\partial W}{\partial \phi} \right)^2 \right) + V(r) = \frac{1}{2m} \left((d_r W_1)^2 + \frac{\alpha_\phi^2}{r^2} \right) + V(r) = E.$$

As an ordinary differential equation, this can be solved by a separation of variables, yielding

$$d_r W_1 = \sqrt{2m(E - V(r)) - \frac{\alpha_\phi^2}{r^2}},$$

and thus

$$W = \int dr \sqrt{2m(E - V(r)) - \frac{\alpha_\phi^2}{r^2}} + \alpha_\phi \phi.$$

Choosing E as the second integration constant, $E = \alpha_1$, yields as new coordinate

$$Q_1 = \frac{\partial W}{\partial \alpha_1} = \frac{\partial W}{\partial E} = \int dr \frac{m}{\sqrt{2m(E - V(r)) - \frac{\alpha_\phi^2}{r^2}}} = \beta_1 + t,$$

where the last equality follows by construction.

The second new variable is then

$$Q_2 = \frac{\partial W}{\partial \alpha_2} = \frac{\partial W}{\partial \alpha_\phi} = \phi - \int dr \frac{\alpha_\phi}{r^2 \sqrt{2m(E - V(r)) - \frac{\alpha_\phi^2}{r^2}}} = \beta_2,$$

¹⁷Unfortunately, there is no better, and especially no more constructive way, than Hamilton-Jacobi theory to find ideal coordinates. This implies that often experience and intuition is invaluable to simplify a mechanical problem.

which is, as a cyclic coordinate, time-independent.

This solves the problem. To compare with the results of section 2.7, identify

$$\begin{aligned}\beta_2 &= \phi_0 \\ x &= \frac{1}{r} \\ \alpha_\phi &= l\end{aligned}$$

yielding

$$\phi = \phi_0 - \int dx \frac{1}{\sqrt{\frac{2m}{l^2} \left(E - V\left(\frac{1}{x}\right) \right) - x^2}}$$

in agreement with (2.20-2.21), if the potential is exchanged for the effective potential of (2.18).

In this case, the usage of the Hamilton-Jacobi equation produced in a straightforward way, somewhat simpler than in section 2.7, the result. However, the usage of the approach may also make problems more involved. As an example, consider the case of a particle in a homogeneous gravity field. The Hamilton function is then

$$H = \frac{1}{2m} p_i^2 + mgz,$$

where the two coordinates x and y are cyclic. An adequate ansatz for the characteristic function is therefore

$$W = W_1(z) + \alpha_x x + \alpha_y y.$$

This yields the Hamilton-Jacobi equation

$$\frac{1}{2m} \left((d_z W_1)^2 + \alpha_x^2 + \alpha_y^2 \right) + mgz = E.$$

As before, this is an ordinary differential equation, which can be solved by separation of variables,

$$W_1 = \int dz \sqrt{2m(E - mgz) - \alpha_x^2 - \alpha_y^2} = c - \frac{1}{3m^2 g} \left(2m(E - mgz) - \alpha_x^2 - \alpha_y^2 \right)^{\frac{3}{2}},$$

where c is an integration constant.

This integration constant is associated with the initial condition for the time, which can again be dropped. Following the program, the new variables are then

$$\begin{aligned}Q_1 &= t + \beta_1 = \frac{\partial W}{\partial E} = -\frac{1}{mg} \sqrt{2m(E - mgz) - \alpha_x^2 - \alpha_y^2} \\ Q_2 &= \beta_2 = \frac{\partial W}{\partial \alpha_x} = x + \frac{\alpha_x}{m^2 g} \sqrt{2m(E - mgz) - \alpha_x^2 - \alpha_y^2} \\ Q_3 &= \beta_3 = \frac{\partial W}{\partial \alpha_y} = y + \frac{\alpha_y}{m^2 g} \sqrt{2m(E - mgz) - \alpha_x^2 - \alpha_y^2}.\end{aligned}$$

This solves the problem completely. Transforming back to the original variables can be done by solving the above expressions for them, leading to

$$x = \beta_2 + \frac{\alpha_x}{m}(t + \beta_1) \quad (5.64)$$

$$y = \beta_3 + \frac{\alpha_y}{m}(t + \beta_2) \quad (5.65)$$

$$z = -\frac{1}{2}g(t + \beta_1)^2 + \frac{2mE - (\alpha_x^2 + \alpha_y^2)}{2m^2g}. \quad (5.66)$$

While this results coincides (necessarily) with (2.4), it seems to be a rather involved way of expressing the movement of a particle under a constant, external force.

This becomes more evident when the generalized, constant coordinates β_i and α_i are exchanged for the initial conditions. For convenience, choose $\vec{x}(0) = \vec{0}$ and $\vec{p}(0) = p_0\vec{e}_x$. The former and (5.64-5.66) imply $\beta_i = 0$. The latter and since F_2 depends on the old coordinates and new momenta implies

$$\begin{aligned} p_x &= \frac{\partial W}{\partial x} = \alpha_x & \stackrel{t=0}{=} p_0 \\ p_y &= \frac{\partial W}{\partial y} = \alpha_y & \stackrel{t=0}{=} 0 \\ p_z &= \frac{\partial W}{\partial z} = \sqrt{2m(E - mgz) - \alpha_x^2 - \alpha_y^2} & \stackrel{t=0}{=} \sqrt{2mE - p_0^2} \stackrel{!}{=} 0, \end{aligned}$$

and the last equation requires $E = p_0^2/(2m)$, as expected and identifying the constant E indeed as the energy at $t = 0$. The final result is thus

$$\begin{aligned} x &= \frac{p_0}{m}t \\ y &= 0 \\ z &= -\frac{gt^2}{2}, \end{aligned}$$

which already looks much more like (2.18).

5.13.3 Connection to the action

In subsection 5.13.1 the generating function was also referred to as Hamilton's action. This is, as the name suggests, due to an intimate connection to the action formalism, as will be shown now.

The solution to the Hamilton-Jacobi equation F_2 is a generating function for a canonical transformation. As such, it follows that

$$\begin{aligned} d_t F_2 &= \frac{\partial F_2}{\partial q_i} \partial_t q_i + \frac{\partial F_2}{\partial P_i} \partial_t P_i + \partial_t F_2 \\ &= p_i \partial_t q_i - H = L. \end{aligned} \quad (5.67)$$

Thus, the total time-derivative of F_2 is just the Lagrange function. Performing an integration over time yields

$$F_2 = \int dt d_t F_2 = \int dt L,$$

and thus F_2 equals almost the usual action S of section 5.1. The only difference is that F_2 is the undetermined integral of the Lagrange function, as long as the initial conditions have not been entered. Thus, F_2 can be considered to create all possible actions for any initial conditions, and therefore providing information on all possible trajectories in phase space.

Unfortunately, this does not help in computing F_2 , as to actually performing the integration requires to know the time-dependence of the generalized coordinates and momenta.

A very similar consideration also applies to the characteristic function W , connecting it to the action for the principle of least action of section 5.5.2. In fact, W is identical to the indefinite action A , since

$$d_t W = \frac{\partial W}{\partial q_i} d_t q_i + \frac{\partial W}{\partial P_i} d_t P_i = p_i d_t q_i,$$

as W is just the time-independent part of F_2 . Integrating yields

$$W = \int p_i d_t q_i dt = \int p_i dq_i,$$

and therefore the action of Maupertius' principle.

It is useful to see this in the case of the example of the harmonic oscillator of section 5.13.2. On the one hand, the Lagrange function for the harmonic oscillator with the used initial conditions is

$$L = T - V = \frac{p^2}{2m} - \frac{m\omega^2}{2} q^2 = E(\sin^2(\omega t) - \cos^2(\omega t)) = 2E \sin^2(\omega t) - E.$$

On the other hand, from (5.67) follows

$$d_t F_2 = \frac{dW}{dq} \frac{dq}{dt} - \alpha = p - \alpha = 2E \sin^2(\omega t) - E,$$

as expected.

5.13.4 Angular and action variables

A particular important special case of Hamilton-Jacobi theory are periodic systems. As has been seen in section 2.6, much can be learned about a periodic system by studying the involved frequencies, rather than the positions of the involved particles. In fact, this

observation generalizes to many systems, especially in quantum physics. It is therefore practically useful to see how these features emerge in general.

Before embarking on this endeavor, it is important to further classify by what is meant by periodicity. In the usual case, a system is considered periodic if a particle comes back to a given position after some fixed period τ . If there are multiple particles involved, the system is only periodic if all the particles come back to a given position after some time τ , even if a subset of particles come back to their original position multiple times during this period.

However, in section 5.7 it has been seen that the concepts of position and momenta are exchangeable, even to much more abstract concepts. In the context of theoretical mechanics, it becomes therefore doubtful to define periodicity just in terms of coordinates. Therefore, it is replaced by the following definition in the case of a single coordinate.

Given a set of canonical conjugated variables q and p , with q a generalized coordinate and p its canonically conjugated momentum. If, for all t some quantity τ , called the period, exists such that

$$\begin{aligned} q(t + \tau) &= q(t) \\ p(t + \tau) &= p(t), \end{aligned}$$

the system is said to be periodic and its trajectory in phase space is closed. This case is called a libration. If, on the other hand

$$\begin{aligned} q(t + n\tau) &= q(t) + nq_0 \\ p(t + \tau) &= p(t) \end{aligned}$$

holds, the system is also said to be periodic with period τ , but this is called a rotation.

An example is given by a pendulum with q being the angle and p its conjugated momenta. If the pendulum does not rotate, but merely swings, this is a libration, as the value of the angle is between some fixed values. If it rotates, the angle is enlarged by $q_0 = 2\pi$ every period. It is therefore, as the name suggests, a rotation.

If the system is described by more than a single set of canonical conjugated momenta, then for each pair a period τ_i can be defined. If the periods τ_i are rational multiples of each other, then the total trajectory in phase space is closed. This case is called proper periodic. If each pair is proper periodic, but the periods have non-rational ratios, the trajectory does not close, and the motion is called of limited periodicity.

In the context of periodic motion it is now useful to define so-called action variables

$$J_i = \oint_{\tau} p_i dq_i,$$

where no summation is performed on the i and the integral symbol indicates that the integral should be taken over a full period.

If the system is fully separable, the action variable takes the form

$$J_i = \oint_{\tau} \frac{dW_i}{dq_i} dq_i = W_i|_t^{t+\tau} = \Delta W_i(\alpha_i),$$

where ΔW_i is thus the change of the action, according to section 5.13.3, due to this set of canonically conjugated variables per period of this pair. This explains the name of the variables, which is even kept beyond the separable case. This value will depend on the α_i , as indicated. Since in the separable case all the variable pairs are independent, this can be solved for the J_i , and therefore it is possible to select $W(q_i, J_j)$ as the set of variables of the characteristic function. Since in the separable case all coordinates are cyclic this implies that the Hamilton function only depends on the J_i . It is therefore possible to write the Hamilton function as a function of the action increments per period, showing again the fundamental importance of the action.

The conjugate variables to the J_i are the new variables given by

$$\omega_i = \frac{\partial W}{\partial J_i},$$

which are called angular variables. Their equations of motion are

$$d_t \omega_i = \frac{\partial h}{\partial J_i} = \nu_i(J_j),$$

and these are the constant frequencies, yielding

$$\omega_i = \nu_i t + \beta_i,$$

which is just the behavior of an ordinary angular variable for conventional periodic movements, explaining the name.

So far, this yielded little more than an application of the Hamilton-Jacobi theory to the case of a periodic motion. However, consider the change of any given angular variable i during the period of some other pair J for the separable case,

$$\Delta_j \omega_i = \oint_{\tau_j} d\omega_i = \oint_{\tau_j} \frac{\partial \omega_i}{\partial q_j} dq_j = \oint_{\tau_j} \frac{\partial^2 W}{\partial q_j \partial J_i} dq_j = \frac{\partial}{\partial J_i} \oint_{\tau_j} \frac{\partial W}{\partial q_j} dq_j = \frac{\partial}{\partial J_i} J_j = \delta_{ij}.$$

This can be understood in the following way: Barring all offsets, any canonical variable has to move exactly the same distance around zero to have a periodic motion. Thus, the difference vanishes, when averaging over many periods, if it is not exactly the same

period. This is, of course, not an average. But an arbitrary period, and therefore the result is equivalent to the average over many periods of the variable j . The speed of movement does not matter. If there would be a second variable with the same period, this information would be redundant and therefore eliminated by the constraints, and it therefore does not appear, and thus only a contribution of the same variable remains.

This also implies

$$\Delta_i \omega_i = 1 = \tau_i \nu_i,$$

with no summation implied. Thus $\nu_i = \tau_i^{-1}$ are the frequencies of the corresponding periodic movements.

Though this seems to be trivial enough at first glance, the real power of the method arises when realizing that it makes it unnecessary to obtain the full solutions to obtain the frequencies only. As noted above, this already delivers a lot of information on a system. This can already be seen when considering the simple harmonic oscillator without external force of section 2.6.

It separated Hamilton-Jacobi equation reads

$$\frac{(d_q W)^2}{2m} + \frac{m\omega^2 q^2}{2} = E.$$

yielding the ordinary differential equation

$$d_q W = \pm m\omega \sqrt{\frac{2E}{m\omega^2} - q^2} = p.$$

It is now not necessary to solve this equation. It merely suffices to note that for a periodic movement the rate of change has to vanish at the inflection points, which have thus the values

$$q_{\pm} = \pm \sqrt{\frac{2E}{m\omega^2}}.$$

The action variable has thus the value

$$J = \oint p dq = 2 \int_{q_-}^{q_+} p dq = 2m\omega \left(\frac{q}{2} \sqrt{\frac{2E}{m\omega^2} - q^2} + \frac{E}{m\omega^2} \sin^{-1} \left(q \sqrt{\frac{m\omega^2}{2E}} \right) \right) \Big|_{q_-}^{q_+} = \frac{2\pi E}{\omega}.$$

This equals, by construction, the Hamilton function

$$h = E = \frac{\omega J}{2\pi}$$

and the relevant frequency is

$$\nu = \frac{\partial H}{\partial J} = \frac{\omega}{2\pi}.$$

Of course, this coincides with the result of section 2.6, but here it was not necessary to find $\phi(t)$ to determine the period and frequency in terms of the parameters of the Hamilton function.

If M of the frequencies are integer multiple of each other then the system is called M -fold degenerate. If M is maximum, i. e. $S - 1$ if there are S frequencies, it is called completely degenerate. If there is M -fold degeneracy then there are M relations

$$n_i^m \nu_i = 0,$$

where m counts the condition and the n_i^m are rational numbers. In case of $S = 1$ the system is considered to be also completely degenerate. Note that by suitable multiplications the rational numbers n_i^m can always be replaced by integer numbers.

This can be used to reduce the number of degrees of freedom to $S - M$. Chose

$$F_2(\omega, \bar{J}) = \sum_{m=1}^M \bar{J}_m n_i^m \omega_i + \sum_{m=M+1}^S \bar{J}_m \omega_m,$$

where the second term is the identity transformation for the independent frequencies. For the M degenerate frequencies the new frequencies are

$$\bar{\nu}_m = n_i^m \nu_i = 0.$$

Thus, all the M degenerate frequencies are now zero. Furthermore, since

$$\bar{\nu}_i = \frac{\partial h}{\partial \bar{J}_i}$$

this implies that the new Hamilton function only depends on the non-degenerate action variables. Thus, degenerate motion does not contain independent information. The action variables associated with non-zero, non-degenerate frequencies are also called eigenaction variables.

One of the basic postulates in the early formulation of quantum physics, the so-called Bohr-Sommerfeld postulate, was that all eigenaction variables can only take values which are integer multiplies of the quantum of action, Planck's constant. With this postulate quantization was build into any (periodic) mechanical system. This postulate was a decisive step in the understanding of the line spectrum of hydrogen. Modern quantum physics supersedes this postulate with more fundamental ones, but a (modified) version of the Bohr-Sommerfeld postulate can then be derived for periodic systems.

Chapter 6

Selected special topics

In this chapter a few selected problems and aspects of theoretical mechanics are discussed using the apparatus developed in the previous chapters. These are somewhat involved problems and concepts, and require a full use of the developed techniques. They should therefore demonstrate the possibilities of what has been achieved up to this point.

6.1 The Kepler problem revisited

To give a challenging and non-trivial application of the Hamilton-Jacobi theory, often considered to be the epitome of theoretical mechanics, consider once more the Kepler problem of section 2.7.3. The Hamilton function reads

$$H = \frac{1}{2m} \left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 \sin^2 \theta} \right) - \frac{k}{r}.$$

In contrast to the examples in section 5.13 this does not seem to be fully separable, since only the coordinate ϕ is cyclic. However, consider its Hamilton-Jacobi equation

$$\frac{2}{2m} \left((\partial_r W)^2 + \frac{(\partial_\theta W)^2}{r^2} + \frac{(\partial_\phi W)^2}{r^2 \sin^2 \theta} \right) - \frac{k}{r} = E.$$

Studying this equation, it is seen that θ has only a single explicit appearance. In this case, this will be sufficient to fully separate the system.

Making the ansatz

$$W = W_r(r) + W_\theta(\theta) + \alpha_\phi \phi,$$

where it was used that ϕ is cyclic, leads, after some rearrangements, to

$$\frac{r^2}{2m} (d_r W_r)^2 - kr - Er^2 = \frac{1}{2m} \left((d_\theta W_\theta)^2 + \frac{\alpha_\phi^2}{\sin^2 \theta} \right).$$

This equation can be separated, as both sides have to be independently equal to a constant, to be called α_θ . Using the expression for the angular momentum in spherical coordinates identifies $\alpha_\theta^2 = \vec{l}^2 = l^2$. At the same time, it was shown that $\alpha_\phi = l_z$. Thus, all three relevant constants have immediate physical implications.

As the motion is periodic, it is useful to determine the action variables next. As in section 5.13.4, the points of inflection can be obtained from the vanishing of derivatives. Consider them separately.

The case of J_ϕ is straightforward, as the coordinate is cyclic. Thus

$$J_\phi = \oint_{\tau_\phi} d_\phi W_\phi = \alpha_\phi \oint_{\tau_\phi} d\phi = 2\pi l_z. \quad (6.1)$$

This is the rotation of the whole plane in which the movement takes place at a constant angular velocity.

The situation for J_θ is a bit more involved. To determine

$$J_\theta = \oint_{\tau_\theta} d_\theta W_\theta d\theta = \oint_{\tau_\theta} \sqrt{l^2 - \frac{l_z^2}{\sin^2 \theta}} d\theta \quad (6.2)$$

requires to determine the points of inflection in θ . They occur whenever the argument of the root vanishes, yielding

$$\sin \theta_\pm = \frac{l_z}{l}.$$

To determine the initial and final points requires to ensure that the root stays real. The ensuing integral is far from trivial, and the result is only cited here¹,

$$\begin{aligned} J_\theta &= 2il_z^2 \int_{\theta_-}^{\theta_+} \frac{\sqrt{1 - \frac{l_z^2}{l^2} \sin^2 \theta}}{\sin \theta} d\theta \\ &= 2il_z^2 \left(-\frac{1}{2} \ln \frac{\sqrt{1 - \frac{l_z^2}{l^2} \sin^2 \theta} + \cos \theta}{\sqrt{1 - \frac{l_z^2}{l^2} \sin^2 \theta} - \cos \theta} + \frac{l_z}{l} \ln \left(\frac{l_z}{l} \cos \theta + \sqrt{1 - \frac{l_z^2}{l^2} \sin^2 \theta} \right) \right) \Bigg|_{\theta_-}^{\theta_+} = 2\pi(l - l_z), \end{aligned}$$

even though the final result is deceptively simple.

An interesting observation so far is that the value of k did not yet play a role. The angular motion is completely independent of it. This is a consequence of the rotational

¹Rather than this brute-force approach, a solution can also be obtained by employing the constancy of each component of angular momentum separately.

symmetry of the problem². Of course, in the end this has to play a role, and it resurfaces now in the equation for J_r ,

$$J_r = \oint_{\tau_r} \sqrt{2m \left(E + \frac{k}{r} \right) - \frac{(J_\phi + J_\theta)^2}{4\pi^2 r^2}} dr = \oint_{\tau_r} \sqrt{2m \left(E + \frac{k}{r} - \frac{l^2}{2mr^2} \right)} dr.$$

As is already known from section 2.7.3, the bounded motion are periodic, and the values r_1 and r_2 between it oscillates can be obtained in the same way as before. The integrand is actually even more cumbersome than before³, and thus only the result will be quoted, which reads

$$J_r = -2\pi l + \pi k \sqrt{\frac{2m}{-E}} = -(J_\theta + J_\phi) + \pi k \sqrt{\frac{2m}{-E}}. \quad (6.3)$$

The appearance of the negative of the energy E should not come as a surprise: Only bounded motions are periodic, and bounded motions have negative energies for a potential energy written as k/r .

With this, the new Hamilton function is obtained as

$$h = -\frac{2\pi^2 m k^2}{(J_r + J_\theta + J_\phi)^2}, \quad (6.4)$$

which only depends on the action variables. That they are added emphasizes that these cannot be considered as the components of a vector. The three frequencies are

$$\nu_i = \frac{\partial h}{\partial J_i} = \frac{4\pi^2 m k^2}{(J_r + J_\theta + J_\phi)^3} \equiv \nu = \frac{1}{\tau} \quad (6.5)$$

and coincide; the system is completely degenerate.

From these investigations Kepler's third law arises as a(n almost) trivial extension. Because of (6.3-6.5) and the (not explicitly stated) value of r_2 it follows that

$$\tau = \pi k \sqrt{\frac{m}{-2E^3}} = 2\pi \sqrt{-\frac{r_2^3 m}{k}}$$

and thus $\tau^2 \sim r_2^2$.

6.2 Spinning top

The treatment of rotating bodies with the Lagrangian and Hamiltonian formalism is often needed. To discuss its features, it is useful to consider a particular example, the so-called spinning top.

²In a more general context, this feature will be reencountered as the Wigner-Eckhart theorem.

³An analytic evaluation is not directly possible, but requires function theory for a solution with reasonable effort.

6.2.1 Euler's angles

A spinning top is a rigid body. It has therefore only six degrees of freedom, three describing the movement of the center of mass, and three describing possible rotations of the body. The movement of the center of mass has nothing to do with the body itself, as discussed in section 2.8, and is rather following the trajectory of a mass point in which all of the mass is concentrated. This leaves the rotation of the body.

The first step is the choice of suitable generalized coordinates. Very useful in this context are Euler's angles. The reason for this is that suitable generalized coordinates need to be independent of each other, as otherwise not all constraints have been eliminated. As will be seen, Euler's angles provide exactly this feature.

They are derived from the fact that any rotation in three dimensions can be described by a sequence of three rotations, as was already used in section 3.1.2. Euler's angles are therefore introduced in the following way: Consider a fixed coordinate system. At every instant in time, the relative orientation of the body is then fixed by three consecutive rotations.

First, rotate by an angle ψ around the original z axis in the coordinate system xzy . This gives a new coordinate system $\xi\eta z$. In this coordinate system, rotate around the ξ axis by an angle θ . This gives a new system $\xi'\eta'\zeta$. Finally, the system is rotated around the ζ axis by an angle ϕ . In terms of the matrices (3.5), a complete rotation reads

$$J = J_1(\phi)J_3(\theta)J_1(\psi),$$

and a vector in the new system is given by $\vec{r}' = J\vec{r}$. The time-dependent position of the vector \vec{r}' in terms of the original position are given by making the angles time-dependent. As an orthogonal transformation, it holds that $\vec{r} = J^T\vec{r}'$. It is useful to require that the fixed coordinate system coincides with the body-fixed system at $t = 0$, i. e. $J(t = 0) = 1$.

A number of interesting results can be deduced from the fact that J is an orthogonal rotation matrix. Given that its determinant is one⁴ at $t = 0$, and that it should be a continuous function of time, its determinant needs to stay one for all times. Furthermore, it has at least one real eigenvalue of value $+1$. But for any real eigenvalue there is a real eigenvector with

$$J(t)\vec{\omega}(t) = \vec{\omega}(t),$$

and thus $\omega(t)$ does not change under J . It is thus the, possibly time-dependent, rotation axis: There is always a fixed rotation axis for any rotation, which is known as Euler's

⁴It could also be -1 , which happens if the two coordinate systems are mirrored with respect to each other.

theorem. The other two eigenvalues can only be real, if $J(t) = 1$, to maintain the value of the determinant at time zero, or both are -1 . Otherwise, they are complex, and therefore do not define a physical eigenvector. If they are -1 , they correspond to the flipped rotation axis, and are therefore nothing new.

6.2.2 The equations of rotation

Start with the Lagrange function. The kinetic energy for a rotation involves, as discussed in section 2.11, the tensor of inertia. Assume that a coordinate system has been chosen in which the tensor of inertia has been brought to its main axis form. Then the Lagrange function reads

$$L = \frac{1}{2} = \frac{1}{2} \left(\sum_i I_i \omega_i^2 \right) - V(\theta, \phi, \psi), \quad (6.6)$$

where the angles are still Euler's angles. The connection of the rotational speed to Euler's angle is given by

$$\vec{\omega} = \begin{pmatrix} \sin \theta \sin \psi \frac{d\phi}{dt} + \cos \psi \frac{d\theta}{dt} \\ \sin \theta \cos \psi \frac{d\phi}{dt} - \sin \psi \frac{d\theta}{dt} \\ \cos \theta \frac{d\phi}{dt} + \frac{d\psi}{dt} \end{pmatrix}.$$

The derivatives of the potential with respect to Euler's angles will in general not be a component of the torque. The exception is ψ , as this is the rotation associated with the fixed z -axis. Thus its Euler-Lagrange equations reads

$$I_3 \frac{d\omega_3}{dt} - \omega_1 \omega_2 (I_1 - I_2) = \frac{d}{dt} \frac{\partial T}{\partial \dot{\psi}} - \frac{\partial T}{\partial \psi} = -\frac{\partial V}{\partial \psi} = M_3. \quad (6.7)$$

The other two equations would have quite a different form. However, it is not necessary to resort to them. Note that the angle actually no longer appears explicitly in the equation of motion, only the generalized speeds. At the same time, the choice of z -axis was arbitrary. Therefore, this could be done by exchanging the axes, leading to

$$I_1 \frac{d\omega_1}{dt} - \omega_2 \omega_3 (I_2 - I_3) = M_1 \quad (6.8)$$

$$I_2 \frac{d\omega_2}{dt} - \omega_1 \omega_3 (I_3 - I_1) = M_2. \quad (6.9)$$

(6.8-6.9) are not the Euler-Lagrange equations of the other Euler angles. Still, they are valid equations of motion, and (6.7-6.9) together are known as Euler's equations.

Euler's equations can actually be solved if the torque vanishes in their full generality in terms of so-called elliptic functions. In fact, even the top's qualitative behavior can be deduced without solving them. However, neither of this is fully transparent, and it is better to study some special cases, to identify the most pertinent features.

6.2.3 Precession

The first interesting case occurs for a symmetric object with $I_1 = I_2$. Then (6.9) implies that ω_3 is constant in time. This allows to eliminate either ω_1 or ω_2 when combining (6.8-6.9). Choosing ω_1 , this is achieved by deriving (6.8) once more with respect to time, yielding

$$I_1 \frac{d^2 \omega_1}{dt^2} = \frac{d\omega_2}{dt} \omega_3 (I_1 - I_3) = -\frac{(I_1 - I_3)^2}{I_1} \omega_3^2 \omega_1.$$

This is the equation of a harmonic oscillator. Likewise, a similar equation arises for ω_2 .

The solution, for suitable initial conditions, is

$$\begin{aligned} \vec{\omega} &= \begin{pmatrix} A \sin(\Omega t) \\ A \cos(\Omega t) \\ \omega_z \end{pmatrix} \\ \Omega &= \frac{I_1 - I_3}{I_1} \omega_z. \end{aligned}$$

The rotation axis therefore rotates itself around the z -axis. This behavior is called precession.

6.2.4 Top in a gravitational field

Consider as a more complicated case again an object with a symmetry axis, but now under the influence of a constant force, and therefore torque. This is the behavior of a (spinning) top in a gravitational field, which in the form of a gyroscope is one of the most important practical applications of this problem.

In this case the Lagrange function (6.6) reduces to

$$L = \frac{I_x}{2} ((d_t \theta)^2 + \sin^2 \theta (d_t \phi)^2) + \frac{I_z}{2} ((d_t \psi) + \cos \theta (d_t \phi))^2 - Mgl \cos \theta,$$

where M is the mass of the top and l is the distance between the point where the top touches the ground and its center of mass on its symmetry axis.

It is immediately seen that both ψ and ϕ are cyclic. This gives two integrals of motions, which are two components of the angular momentum,

$$\begin{aligned} p_\psi &= \frac{\partial L}{\partial d_t \psi} = I_z (d_t \psi + \cos \theta d_t \phi) = I_3 \omega_z = I_x a \\ p_\phi &= \frac{\partial L}{\partial d_t \phi} = (I_x \sin^2 \theta + I_z \cos^2 \theta) d_t \phi + I_z \cos \theta d_t \psi = I_x b, \end{aligned}$$

where the recasting in terms of new constants a and b will simplify calculations below. Since the system is conservative, also the energy is constant,

$$E = T + V = \frac{I_x}{2} ((d_t\theta)^2 + \sin^2\theta (d_t\phi)^2) + \frac{I_z}{2}\omega_z^2 + Mgl \cos\theta.$$

This leaves only three quantities, the three angles as a function of time, to be determined.

Fortunately, it is possible to use the three integrals of motion for that, and therefore only differential equations of first order need to be solved. The first step is to single out $d_t\phi$ from the combination of equations, yielding

$$d_t\phi = \frac{b - a \cos\theta}{\sin^2\theta}, \quad (6.10)$$

and thus ϕ can be obtained from θ . Similarly,

$$d_t\psi = \frac{I_x a}{I_z} - \frac{b - a \cos\theta}{\sin^2\theta} \cos\theta, \quad (6.11)$$

and thus also ψ is known once θ is.

Fortunately, it is possible to combine the three integrals of motion such that an equation involving only θ is obtained, reading

$$\begin{aligned} (d_t\theta)^2 \sin\theta &= \sin^2\theta (\alpha - \beta \cos\theta) - (b - a \cos\theta)^2 \\ \alpha &= \frac{2 \left(E - \frac{I_z \omega_z^2}{2} \right)}{I_x} \\ \beta &= \frac{2Mgl}{I_x}. \end{aligned}$$

This equation can be solved by direct integration if the substitution

$$u = \cos\theta \quad (6.12)$$

is performed, leading to

$$t - t_0 = \int_{u(t_0)}^{u(t)} \frac{du}{\sqrt{(1-u^2)(\alpha - \beta u) - (b - au)^2}}. \quad (6.13)$$

Thus, the problem is fully solved by the equations (6.10), (6.11), and (6.13). While this integral can be solved using elliptic functions, the final result is once more not very instructive.

However, similar to the case of the central potential in section 2.7, it is possible to read off the qualitative behavior already without performing the integral explicitly. For this, it is useful to consider the differential form of (6.13), reading

$$(d_t u)^2 = (1 - u^2)(\alpha - \beta u) - (b - au)^2.$$

The right-hand-side is a polynomial of third order. Because the left-hand-side is positive, as are the constants α and β , this implies that the right-hand-side goes to $\pm\infty$ for $u \rightarrow \pm\infty$. Furthermore, because of (6.12), only the interval $-1 \leq u \leq 1$ is relevant. If $u = \pm 1$, the right-hand-side is necessarily negative or zero. This implies that there are necessarily three real roots. If both are negative, this implies that one of the roots has to be at a location $u > 1$, and therefore plays no role. If both are zeros, this actually corresponds to the fact that $\theta = \pi/2$, and the top is upright. Since the roots are the points of reflection, as there the rate of change of u vanishes, this implies that u can move in general such that $-1 < \cos \theta < 1$, and therefore the top's symmetry axis cannot fall to the floor.

Considering the curves which the symmetry axis exhibits, there are three possibilities. One is that the symmetry axis always moves forward in θ , and rotates around the direction of gravity. This is the precession of section 6.2.3. However, since the other angles also moves, a second movement overlays with this. One is that the symmetry axis oscillates up and down in some range. This is called a nutation, and thus the total effect is called precession-nutation.

Alternatively, it can move not only forwards, but also backwards in θ , and the rotation axis performs loops due to the nutation. Finally, there is a limiting case between both other options, where the loop degenerates to a point, giving an edge in the path of the rotation axis.

This can be made more quantitative, without actually solving (6.13), in various limits, e. g. if the spin has much more or much less kinetic energy than potential energy. This is particularly important for practical application, as it leads to closed expression for the frequencies of the movements as a function of the gravitational field, and therefore can also give information on geographical position. This leads beyond the scope of this lecture.

6.3 Continuum mechanics

Many systems in mechanics contain a very large number of point particles. In many of these cases it becomes suitable to deal with these particles rather in terms of density than of the individual particles, as already hinted at in section 2.8. In this case, matter is considered as a continuum, described by a mass density $\rho(\vec{r})$. This is the purview of continuum mechanics.

6.3.1 Systems of many oscillators

Before actually treating matter as a continuum system, it is very helpful to first consider a very special system with many degrees of freedom, that of many (coupled) oscillators.

Such systems in themselves are relevant, as many physical systems can be described by them, especially in solid state physics. Furthermore, taking the limit of an infinite number of these oscillators already provides a good description of many continuum systems, and it is therefore technically useful to first study a finite, but large, such system. Moreover, according to section 2.9, any system close to a stable equilibrium is also described by a system of many oscillators.

For this to happen, it is not necessary that the system is described in position space coordinates. Also in generalized coordinates stable equilibria are encountered, if there is a minimum of the potential in terms of the generalized coordinates. It is then also possible to expand the potential in a Taylor series in the generalized coordinates. Taking for N generalized coordinates q_i the values q_i^0 to be the equilibrium position, it is then useful to introduce the fluctuation coordinates

$$\eta_i = q_i - q_i^0.$$

Moreover, if the system should remain close to equilibrium also the kinetic energy needs to be close to zero. Considering only conservative systems with the kinetic energy a quadratic function in the generalized speeds, the total Lagrange function reads

$$\begin{aligned} L &= m_{ij} \frac{d\eta_i}{dt} \frac{d\eta_j}{dt} - V_{ij} \eta_i \eta_j \\ V_{ij} &= \left. \frac{\partial^2 V}{\partial q_i \partial q_j} \right|_{q_i=q_i^0, q_j=q_j^0}, \end{aligned}$$

where the constant term in the potential has been dropped and it was permitted that the kinetic term has also off-diagonal elements in the generalized coordinates. The Euler-Lagrange equations are

$$m_{ij} \frac{d^2 \eta_j}{dt^2} + V_{ij} \eta_j = 0, \quad (6.14)$$

and therefore form a set of N coupled differential equations. Fortunately, this type of coupled differential equations can be solved in closed form.

Because each individual equation has the same form as an harmonic oscillator, an ansatz of type

$$\eta_i = \Re(a_i e^{-i\omega t})$$

appears as a reasonable starting point. Intentionally here only the same frequency is used for the whole set of oscillators. This is based on the insight from section 2.6 that an harmonic oscillator under an external influence starts to behave like the external influence. Thus, it appears possible that there are common oscillations of all oscillators. The different

possible solutions will eventually be found to be different values for ω , which then can be superposed to find arbitrary solutions.

This turns the system of differential equations (6.14) into a set of linear equations for the amplitude factors a_i ,

$$V_{ij}a_j - m_{ij}\omega^2 a_j = 0. \quad (6.15)$$

Such a system of equations has only a solution if the determinant of the matrix

$$B_{ij} = V_{ij} - m_{ij}\omega^2 \quad (6.16)$$

vanishes, which follows from the general theory of linear systems. This gives an N th order polynomial for the frequency ω , which thus yields $2N$ solutions, every time $\pm\omega$, producing all the solutions. Especially, also the complex solutions are admissible, as these will be exponentially damped or enhanced (unstable) oscillations⁵. The amplitudes are the solutions to this homogeneous system, which implies that one of the (non-vanishing) amplitudes will be arbitrarily selectable, and the remaining follow from the solutions of the linear system.

An interesting reinterpretation is possible if the mass matrix is diagonal, $m_{ij} = m_i\delta_{ij}$, with no summation implied. Rescaling the η_i by m_i , the masses drop out, and the problem takes the form of an eigenvalue problem,

$$V\vec{a} = \lambda\vec{a},$$

where $\lambda = \omega^2$ are the eigenvalues. Furthermore, Newton's third law requires that the V are symmetric. This implies that all eigenvalues are real, and thus the so-called eigenfrequencies ω^2 are either purely real or purely imaginary. The vectors of amplitudes are then the eigenvectors of the matrix V , and form a complete basis and are orthogonal with respect to each other. These amplitudes are also called eigenoscillations of the system. Note that this also implies that there exists an orthogonal transformation, which is necessarily also a canonical transformation, which decouples all oscillators, as any symmetric matrix can be diagonalized.

If the matrix m is not diagonal, it is possible to construct a very similar line of reasoning, ultimately leading to equivalent results. In this case, it is possible to reinterpret the problem as a problem in a space which is not Euclidean, but rather has a metric m . In the end, the result are again $2N$ eigenvalues $\pm\omega_k$ and N eigenvectors \vec{a} with arbitrary norm in this metric.

If there are degenerate eigenvalues, the eigenspaces to a given eigenvector are not one-dimensional. In these cases it is necessary to construct a basis within these eigenspaces.

⁵The latter will not appear, if the initial assumption of a system in equilibrium is not violated.

In the end, the total dimensionality does not change, and therefore also in this case all solutions to (6.14) can be constructed in the same way⁶.

It should be noted that the eigenvectors determine the relative ratio of the amplitudes of the oscillators, but not the absolute value. The general solution will therefore be

$$\eta_i = \Re \sum_k a_i^k (C_k^+ e^{i\omega_k t} + C_k^- e^{-i\omega_k t}) = \sum_k a_i^k f_k \cos(\omega_k t + \delta_k),$$

where $2N$ undetermined constants remain, either in the form of some combination of real and imaginary parts of C_k^\pm or as amplitude factors f_k and phase shifts δ_k . They belong to every of the N oscillations, and are determined by the initial conditions. For each of these oscillations the eigenvectors \vec{a} determine the relative amplitudes of the oscillators. These are a property of the system, and are not determined by any initial conditions. It is very important to make this distinction carefully. Note that the motion may be proper periodic if all the frequencies have rational ratios, or may be only of limited periodicity, if this is not the case.

It is useful to introduce normal coordinates. Define the matrix

$$A_{ij} = a_i^j$$

from the normalized eigenvectors \vec{a}^k of B , and define the normal coordinates ζ such that

$$\begin{aligned} \vec{\eta} &= A\vec{\zeta} \\ \vec{\zeta} &= A^{-1}\vec{\eta}, \end{aligned}$$

The eigenvectors \vec{a}^k of a symmetric matrix form an orthonormal base. The matrix A is therefore orthogonal, and this also implies that the inverse exist and that $A^{-1} = A^T$. Furthermore, any orthogonal matrix defines a coordinate transformation, especially a rotation. Therefore, the normal coordinates are again a set of generalized coordinates, as any rotation in configuration space is a canonical transformation, if also the generalized speeds are transformed accordingly. By construction, this matrix also diagonalizes V to its diagonal form,

$$\lambda = AVA^T,$$

where the matrix λ has the eigenvalues $\lambda_k = \omega_k^2$ as entries. In the equilibrium case it is therefore a positive semi-definite matrix.

⁶Note that there can be no more than $2N$ solutions, as guaranteed by the mathematical theorem on ordinary differential equations. Therefore having constructed all $2N$ solutions, one can be sure that all solutions have been captured. If this would have been rather a partial differential equation, a similar statement is in general not possible.

This implies that it is possible to rewrite the Lagrange function as

$$L = \frac{1}{2} \left(\frac{\vec{\eta}}{dt} \right)^T M \frac{d\vec{\eta}}{dt} - \frac{1}{2} \vec{\eta}^T V \vec{\eta} = \frac{1}{2} \left(\frac{\vec{\zeta}}{dt} \right)^T \frac{d\vec{\zeta}}{dt} - \frac{1}{2} \vec{\zeta}^T \lambda \vec{\zeta},$$

where a rescaling of the fluctuations η by the mass has been performed. This is actually also possible if the matrix M is not diagonal and scaled out, though orthogonality and rotations have then to be defined with respect to a metric M . Important here is, however, only that it is always possible to recast the Lagrange function in this form.

Geometrically, this transformation rotated into the coordinate system created by the eigenvectors. Thus, in normal coordinates all oscillations of the ζ decouple, and the system is described by N decoupled oscillators, every oscillating according to the corresponding eigenfrequency ω_k^2 . Comparison to section 5.13.4 shows that this is also the form which would be obtained after applying Hamilton-Jacobi theory to the system. In these coordinates every oscillations is also called normal oscillation.

As the full movement is now given by a composition of normal oscillations as dictated by the initial conditions, it is possible to consider the physical picture: The system is able to perform a number of movements, the normal oscillations. Depending on the initial conditions, any number of these normal oscillations can be excited, but only movements are possible which can be decomposed into normal oscillations. The system is only able to respond in a certain, quasi-quantized form. This picture is very helpful when introducing continuous systems, electromagnetism or other field theories, and also quantum systems.

It is useful to consider an explicit example. Take e. g. three particles, connected by two springs with the same strength k , all confined to a linear motion in one dimension. The particles at the ends should have a mass m and the one in the center a mass M . If the length of the springs is a , the potential energy is

$$V = \frac{k}{2}(x_2 - x_1 - a)^2 + \frac{k}{2}(x_3 - x_2 - a)^2.$$

As the equilibrium position⁷ will be that the springs are at the normal length a , the difference between the equilibrium positions is also a , and in terms of the fluctuations η_i the potential energy takes the form

$$V = \frac{k}{2}(\eta_2 - \eta_1)^2 + \frac{k}{2}(\eta_3 - \eta_2).$$

⁷In the present case, strictly speaking, there would be no need to consider equilibrium positions, as the potential is already of harmonic oscillator form. For the sake of sticking with the developed procedures this will be done nonetheless.

The corresponding kinetic energy is

$$T = \frac{m}{2} ((d_t \eta_1)^2 + (d_t \eta_3)^2) + \frac{M}{2} (d_t \eta_2)^2.$$

The matrix B from (6.16) is then

$$B = \begin{pmatrix} k - \omega^2 m & -k & 0 \\ -k & 2k - \omega^2 M & -k \\ 0 & -k & k - \omega^2 m \end{pmatrix}.$$

This form - elements on the diagonal and otherwise only elements on directly adjacent subdiagonal, is characteristic for a one-dimensional system of springs, where only nearest neighbors are connected. Thus, the behavior obtained in the following is qualitatively already rather characteristic of such systems. Such systems play a certain role in many physical contexts, especially in solid state physics and optical lattices.

The next step is to solve the equation

$$0 = \det B = \omega^2 (k - \omega^2 m) (k(M + 2m) - \omega^2 M m)$$

for ω^2 . There are three solutions,

$$\begin{aligned} \omega_1 &= 0 \\ \omega_2 &= \sqrt{\frac{k}{m}} \\ \omega_3 &= \sqrt{\frac{k}{m} \left(1 + \frac{2m}{M}\right)}. \end{aligned}$$

The first frequency appears somewhat odd, as this would be no oscillation at all. However, there is a comparatively simple explanation for it. This is a uniform motion of the whole system in either direction. Since the constraints do not forbid it, this is a consistent solution. This could have been excluded by adding a constraint that, say, the center-of-mass coordinate needs to be fixed. This would have reduced the degrees of freedom from three to two, leaving only non-vanishing frequencies.

The next step is to solve (6.15) to find the relative sizes, i. e. solve $B\vec{a}^k = 0$. This is an ordinary system of linear equations, which yields the (normalized) solutions

$$\vec{a}^1 = \frac{1}{\sqrt{2m+M}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \vec{a}^2 = \frac{1}{\sqrt{2m}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \quad \vec{a}^3 = \begin{pmatrix} \frac{1}{\sqrt{2m(1+\frac{2m}{M})}} \\ \frac{-2}{\sqrt{2M(2+\frac{M}{m})}} \\ \frac{1}{\sqrt{2m(1+\frac{2m}{M})}} \end{pmatrix}.$$

where the normalization is chosen for later convenience. The first case is indeed a collective motion in one direction. The second is an oscillation of the endpoints with respect to a fixed center. The third is a relative oscillation of the center mass with respect to the two other masses, which leaves also the center of mass fixed.

Generalizing to masses connected by effective springs in three dimensions, one lesson is that always the motion of the center of mass will appear, if not constrained. Thus, there will always be $3N - 3$ non-trivial eigenfrequencies. Further degeneracies will occur if the system shows a symmetry, as then the symmetry transformation needs to leave the motion unchanged. The non-trivial, non-degenerate eigenfrequencies then fully characterize the system. However, in general it will become more involved to determine them, as it requires to solve an $3N - 3$ order polynomial, which is in general not possible in closed form.

It is possible to extend the present treatment to generalize the full case with dissipation and external driving forces, as in section 2.6. This leads to no new conceptual insights, and will therefore not be done here.

6.3.2 Continuous systems of oscillators

After this preliminary investigation, it is now possible to go to continuous systems.

As a next step consider again the linear chain, but now admit an (arbitrarily large) number N of particles, but which should all have the same mass. The Lagrange function is then given by

$$L = \sum_i \left(\frac{m}{2} (d_t \eta_i)^2 + \frac{k}{2} (\eta_{i+1} - \eta_i)^2 \right).$$

In principle, there need to be some additional terms to take care of boundary terms. However, they will not play a role, especially as later the limit $N \rightarrow \infty$ will be taken. If now the equilibrium distance between any two particles is equal and of size a , this can be rewritten as

$$L = \sum_i a \left(\frac{m}{2a} (d_t \eta_i)^2 + \frac{ka}{2} \left(\frac{\eta_{i+1} - \eta_i}{a} \right)^2 \right) = \sum_i a L_i$$

The quantity $m/a = \mu$ is the mass density of the system. The quantity ka has no direct interpretation. If the connection is indeed in the form of springs, it turns out that for usual springs this product is constant, as a short spring has a larger spring constant, the so-called module of Young Y . Here, it will be required by definition that $ka = Y$, just like m/a , is held constant for any value of a .

Now label the particles not by a discrete index, but rather by their position, i. e. $\eta(x)$ is the displacement of the particle with equilibrium position x against its equilibrium

position. Then

$$\frac{\eta_{i+1} - \eta_i}{a} = \frac{\eta(x+a) - \eta(x)}{a} \xrightarrow{a \rightarrow 0} \frac{d\eta}{dx},$$

i. e. the difference in fluctuations becomes in the limit of smaller and smaller distance a of the particles the derivative, or rate of change, in the displacement η . At the same time the sum becomes a Riemann sum, leading to

$$L = \int dx (\mu(d_t\eta)^2 - Y(d_x\eta)^2) = \int dx \mathcal{L}(x),$$

where \mathcal{L} is called the Lagrangian density. Likewise, the equation of motion turns from

$$m d_t^2 \eta_i - k(\eta_{i+1} - 2\eta_i + \eta_{i-1}) = 0$$

to

$$\mu d_t^2 \eta(x) - Y d_x^2 \eta = 0 \tag{6.17}$$

which is now an equation for the function $\eta(x, t)$ of two variables, rather than for the finite number of quantities $\eta_i(t)$.

6.3.3 Continuous systems

The previous section outlined everything necessary to define the Lagrange formulation for continuous system. Given a field $\eta(\vec{r}, t)$, the Lagrange function is given by a volume integral over the Lagrange density \mathcal{L} , sometimes called just Lagrangian,

$$L = \int d^3\vec{r} \mathcal{L}(\partial_i \eta, \partial_t \eta, \vec{r}, t)$$

which can now depend explicitly on both time and the space coordinate. For the Lagrange function to be scalar, the Lagrange density needs to be a density. At the current time, η is itself also a scalar under rotations. However, it would also be possible to define vector fields or fields of even higher tensors, and indeed this will already in classical electromagnetism be necessary. However, for simplicity here only scalar fields will be considered.

The action is still a time-integral over the Lagrange function,

$$S = \int dt L = \int dt d^3\vec{r} \mathcal{L},$$

and thus a space-time integral over the Lagrange density. This already suggests that an extension to special relativity is rather straight-forward, and assigns in such a context the Lagrange density a more fundamental role than the Lagrange function.

However, an important difference now occurs when considering virtual displacements. So far, these have been applied to the coordinate at fixed time. Now, however, the elementary degree of freedom is the field rather than the coordinates. Thus, virtual displacements modify the field, $\eta \rightarrow \eta + \delta\eta$, at fixed time and coordinates. At the same time it is now necessary to consider also the changes in direction, not only in time, of the field. Thus, a variation of the Lagrange density under a virtual displacement reads⁸

$$\delta\mathcal{L} = \frac{\partial\mathcal{L}}{\partial\eta}\delta\eta + \frac{\partial\mathcal{L}}{\partial\partial_t\eta}\delta\partial_t\eta + \frac{\partial\mathcal{L}}{\partial\partial_i\eta}\delta\partial_i\eta. \quad (6.18)$$

In very much the same manner as in section 5.1 it is now possible to derive Euler-Lagrange equations by requiring $\delta S = 0$, which implies

$$\int dt d^3\vec{r} \delta\mathcal{L} = 0. \quad (6.19)$$

To rewrite all contributions in terms of $\delta\eta$ note that the variations at the boundaries vanish, as in section 5.1.2. Thus, derivatives can be moved around freely. Then

$$\begin{aligned} \int dt \frac{\partial\mathcal{L}}{\partial\partial_t\eta} \delta\partial_t\eta &= \int dt \frac{\partial\mathcal{L}}{\partial\partial_t\eta} \partial_t\delta\eta = - \int dt \delta\eta \frac{d}{dt} \frac{\partial\mathcal{L}}{\partial\partial_t\eta} \\ \int dt \frac{\partial\mathcal{L}}{\partial\partial_i\eta} \delta\partial_i\eta &= \int dt \frac{\partial\mathcal{L}}{\partial\partial_i\eta} \partial_i\delta\eta = - \int dt \delta\eta \frac{d}{dr_i} \frac{\partial\mathcal{L}}{\partial\partial_i\eta}. \end{aligned}$$

Some comment is in order concerning the appearance of total and partial derivatives. The field η does only depend explicitly on the coordinates and the time, but the coordinates and time do no longer depend also on any other quantities. Thus, total and partial derivatives coincide in this case. However, the Lagrange density can depend on them explicitly. It is thus necessary to take this into account when performing a partial integration, which leads to the requirement to perform a total derivative. This has nothing to do with physics, but only something with performing partial derivatives. Integration and differentiation do only invert each other for full derivatives, not partial derivatives,

$$\begin{aligned} a(\eta(x), x) \eta(x) \Big|_1^2 &= \int_1^2 dx \frac{d}{dx} (a(\eta(x), x) \eta(x)) = \int_1^2 dx \left(\frac{da}{dx} \eta + a \frac{d\eta}{dx} \right) \\ &= \int_1^2 dx \left(\frac{\partial a}{\partial x} \eta + \frac{\partial a}{\partial \eta} \frac{\partial \eta}{\partial x} \eta + a \frac{\partial \eta}{\partial x} \right) \neq \int_1^2 dx \frac{\partial}{\partial x} (a(\eta(x), x) \eta(x)) = \int_1^2 dx \left(\frac{\partial a}{\partial x} \eta + a \frac{\partial \eta}{\partial x} \right). \end{aligned}$$

The last term is not a total differential, and can therefore not be directly integrated.

⁸For simplicity now $\partial_t = \partial/\partial t$ and $\partial_i = \partial/\partial x_i$ will be used as abbreviations.

Returning to (6.18-6.19) then leads to

$$\int dt d^3\vec{r} \left(\frac{\partial \mathcal{L}}{\partial \eta} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \partial_t \eta} - \frac{d}{dr_i} \frac{\partial \mathcal{L}}{\partial \partial_i \eta} \right) \delta \eta = 0.$$

Just as in section 5.1.2 the continuum Euler-Lagrange equations can now be read off

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \partial_t \eta} + \frac{d}{dr_i} \frac{\partial \mathcal{L}}{\partial \partial_i \eta} - \frac{\partial \mathcal{L}}{\partial \eta} = 0, \quad (6.20)$$

which are the dynamical equations governing continuum mechanics. Note that this form is already Lorentz covariant, provided both η and \mathcal{L} are Lorentz scalars, and can then be written as

$$\frac{d}{dx_\mu} \frac{\partial \mathcal{L}}{\partial \partial_\mu \eta} - \frac{\partial \mathcal{L}}{\partial \eta} = 0.$$

This is one of the reasons the Lagrangian formulation is particularly useful for relativistic problems.

It is sometimes useful to define a functional derivative

$$\frac{\delta F[\eta, \vec{r}]}{\delta \eta} = \frac{\partial f}{\partial \eta} - \frac{d}{dr_i} \frac{\partial f}{\partial \partial_i \eta} \quad (6.21)$$

where

$$F = \int d^3\vec{r} f(\eta, \vec{r})$$

implying that the Euler-Lagrange equations can be written as

$$\frac{d}{dt} \frac{\delta L}{\delta \partial_t \eta} - \frac{\delta L}{\delta \eta}$$

where use has been made of the fact that \mathcal{L} does not depend on $\partial_t \partial_i \eta$. This can be generalized to a functional calculus, which is of eminent importance in quantum field theory, but of more limited use, except for making expressions more compact, in classical mechanics.

In this case, both space and time appear on equal footing. As η is now a function, this is a functional differential equation, yielding a partial differential equation for η in its four variables. It is therefore substantially more complicated as the point-particle case, where only a set of functions of a single variable needed to be solved. If there is more than one field involved, this generalizes to a set of such partial differential equations, one for each field.

6.3.4 Applications of the Lagrange formulation

Consider again the problem of section 6.3.2. Its Lagrangian density was

$$\mathcal{L} = \frac{1}{2} (\mu(\partial_t \eta)^2 - Y(\partial_x \eta)^2).$$

The corresponding derivatives are

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \partial_t \eta} &= \mu \partial_t \eta \\ \frac{\partial \mathcal{L}}{\partial \partial_x \eta} &= -Y \partial_x \eta \\ \frac{\partial \mathcal{L}}{\partial \eta} &= 0. \end{aligned}$$

Its Euler-Lagrange equation is therefore

$$\mu \partial_t^2 \eta - Y \partial_x^2 \eta = 0, \quad (6.22)$$

which coincides with (6.17). This is a one-dimensional wave equation with the solutions

$$\begin{aligned} \eta &= \Re \left(c_1 e^{i \frac{vt-x}{x_0}} + c_2 e^{-i \frac{vt-x}{x_0}} \right) \\ v &= \sqrt{\frac{Y}{\mu}}, \end{aligned}$$

which describe forward and backward propagating waves.

To study a more complex problem consider a fluid or gas. Consider now it to be slightly disturbed, on which it reacts with some movement in the three spatial directions. This movement field, what is perceived as sound, is given by a vector field $\vec{\eta}$, which gives at every point in space (and time) the displacement of the medium. The kinetic energy is therefore

$$T = \frac{\mu}{2} (d_t \vec{\eta})^2,$$

where μ is again the density. In Principle, this density would need to be also a field. Here, however, the case of only small distortions will be considered, such that the mass density can be taken to be approximately constant. Without proof, the potential energy, which is essentially sustained by the presence of the medium, and thus how the other particles oppose the movement of a particle, is given by

$$V = \gamma P (\vec{\partial} \vec{\eta})^2 - 2P \vec{\partial} \vec{\eta}$$

where P is the equilibrium pressure and γ characterizes how the medium's pressure reacts to changes of volume. Here, this only motivates why this particular case could be of

practical interest. But the focus is how to treat this system, not where it comes from. This is the purview of a thermodynamic lecture.

The Lagrangian density is therefore

$$\mathcal{L} = T - V = \frac{\mu}{2}(\partial_t \vec{\eta})^2 - \gamma P(\vec{\partial} \vec{\eta})^2 + 2P \vec{\partial} \vec{\eta}.$$

To obtain the equations of motions requires the following quantities

$$\begin{aligned} \frac{\partial(\partial_t \vec{\eta})^2}{\partial \partial_t \eta_i} &= 2\partial_t \eta_i \\ \frac{\partial \vec{\partial} \vec{\eta}}{\partial \partial_i \eta_j} &= \delta_{ij} \\ \frac{\partial(\vec{\partial} \vec{\eta})^2}{\partial \partial_i \eta_j} &= 2\delta_{ij} \vec{\partial} \vec{\eta} \\ \frac{\partial \mathcal{L}}{\partial \eta_i} &= 0. \end{aligned}$$

Interestingly, this result implies that the term linear in $\vec{\partial} \vec{\eta}$ does not contribute to the movement. This is a generic statement: Terms linear in derivatives of the fields do not alter the movement. However, e. g., if the energy stored in the system should be determined, it cannot be ignored.

The equations of motion are thus

$$\mu \partial_t^2 \vec{\eta} - \gamma P \vec{\partial} (\vec{\partial} \vec{\eta}) = 0. \quad (6.23)$$

This is not yet a simply solvable system. To make progress, define the scalar quantity

$$\sigma = -\vec{\partial} \vec{\eta},$$

which is the directed rate of change. As the system is essentially isotropic, it make sense that there will be only one relevant direction, and therefore a single scalar field should actually be sufficient to solve the problem. To rewrite the problem in this form, act with $\vec{\partial}$ on the equation of motion (6.23), yielding

$$\partial^2 \sigma - \frac{\mu}{\gamma P} \partial_t^2 \sigma = 0.$$

Just as before, (6.22), this is a wave equation, with a speed depending on the properties of the gas and its pressure. The rate of change of the movement of the gas therefore forms waves. This is as expected: Sound is an oscillatory wave.

6.3.5 Hamilton formulation

The Lagrange formulation for continuous systems treats space and time on very much equal footing. What is then about the Hamilton formulation, which always uses time as a particular quantity? Can it be useful?

To reach the Hamilton formulation from the Lagrange formulation of section 6.3.3 requires to define the canonical momenta for a field. This is, of course, also a field, the so-called momentum density π . In analogy to section 4.6 define

$$\pi = \frac{\partial \mathcal{L}}{\partial \partial_t \eta} = \frac{\delta L}{\delta \partial_t \eta},$$

which makes only reference to the time-derivative, and therefore breaks the equal treatment of the Lagrange formulation. Of course, if there are multiple fields there will be for each field an own momentum density.

Define then, as in section 5.4, a Hamilton density, or just Hamiltonian,

$$\mathcal{H} = \pi d_t \eta - \mathcal{L}.$$

Just as with the Lagrange function, the Hamilton function is a volume integral of the Hamilton density

$$H = \int d^3 \vec{r} (\pi d_t \eta - \mathcal{L}).$$

Just as with the Lagrange case, it is sufficient to trace out the steps of section 5.4 using fields and also derivatives with respect to the coordinates to find the corresponding equations of motion. Skipping these details leads to the continuum Hamilton equations of motion,

$$-\partial_t \pi = \frac{\delta H}{\delta \eta} = \frac{\partial \mathcal{H}}{\partial \eta} - \frac{d}{dx_i} \frac{\partial \mathcal{H}}{\partial \partial_i \eta} \quad (6.24)$$

$$\partial_t \eta = \frac{\delta H}{\delta \pi} = \frac{\partial \mathcal{H}}{\partial \pi} \quad (6.25)$$

$$\frac{\partial \mathcal{H}}{\partial t} = \frac{\partial \mathcal{L}}{\partial t}. \quad (6.26)$$

In comparison to (6.20) the difference between the Hamilton and the Lagrange formulation becomes now manifest: Derivatives with respect to the momentum density, which are defined using a time-derivative, differ in the absence of spatial derivatives from those of derivatives with respect to the fields themselves. Especially in the context of special relativity the Hamilton formulation is not manifestly covariant, though of course it is still correct. Only more tedious in most cases.

As an example, consider the gas or fluid of section 6.3.4. The momentum density is

$$\pi_i = \frac{\partial \mathcal{L}}{\partial \partial_t \eta_i} = \mu \partial_t \eta_i.$$

The Hamilton density is

$$\mathcal{H} = \vec{\pi} \vec{\eta} - \mathcal{L} = \frac{\vec{\pi}^2}{2\mu} + \frac{P\gamma}{2} (\vec{\partial} \vec{\eta})^2,$$

where the irrelevant linear term has been skipped, even though it would be needed to interpret the Hamilton density as the energy density of the system.

The corresponding equations of motion are

$$\begin{aligned} \partial_t \vec{\eta} &= \frac{\vec{\pi}}{\mu} \\ \partial_t \vec{\pi} &= \vec{\partial} \left(P\gamma \vec{\partial} \vec{\eta} \right), \end{aligned}$$

which are, of course, equivalent to the Lagrange case, and lead to the same result.

Most of the formal developments of chapter 5 can be repeated for the continuous case essentially completely analogous. As an important example consider the continuum version of the evolution equation (5.43). Given some function G , which is a volume integral of a density \mathcal{G} depending on the field and momentum density,

$$G = \int d^3 \vec{r} \mathcal{G},$$

consider its total time derivative. It takes the form

$$\begin{aligned} \frac{dG}{dt} &= \int d^3 \vec{r} \left(\frac{\partial \mathcal{G}}{\partial \eta} \partial_t \eta + \frac{\partial \mathcal{G}}{\partial \partial_i \eta} \partial_i \partial_t \eta + \frac{\partial \mathcal{G}}{\partial \pi} \partial_t \pi + \frac{\partial \mathcal{G}}{\partial \partial_i \pi} \partial_i \partial_t \pi + \frac{\partial \mathcal{G}}{\partial t} \right) \\ &= \int d^3 \vec{r} \left(\left(\frac{\partial \mathcal{G}}{\partial \eta} - \frac{d}{dx_i} \frac{\partial \mathcal{G}}{\partial \partial_i \eta} \right) \partial_t \eta + \left(\frac{\partial \mathcal{G}}{\partial \pi} - \frac{d}{dx_i} \frac{\partial \mathcal{G}}{\partial \partial_i \pi} \right) \partial_t \pi + \frac{\partial \mathcal{G}}{\partial t} \right), \end{aligned}$$

where partial integrations have been performed. Comparing this expression with (6.24-6.26) and the definition of the functional derivative (6.21) permits to rewrite this as

$$\frac{dG}{dt} = \int d^3 \vec{r} \left(\frac{\delta G}{\delta \eta} \frac{\delta H}{\delta \pi} - \frac{\delta G}{\delta \pi} \frac{\delta H}{\delta \eta} \right) + \frac{\partial G}{\partial t} = \{G, H\} + \frac{\partial G}{\partial t}$$

which defines also the continuum version of the Poisson brackets.

6.4 Chaos

A particular subclass of physical systems are those which exhibit a so-called chaotic behavior. Chaotic behavior is best defined in phase space. Given two trajectories at some

point in phase space at some time t , it is possible to define an Euclidean distance between two trajectories as

$$d(t) = (q_i^1 - q_i^2)^2 + (p_i^1 - p_i^2)^2.$$

A system is said to show chaotic behavior if the distance increases exponential (or faster) as a function of time⁹,

$$d(t) \sim e^{at}, \quad (6.27)$$

where a is some constant characteristic of the system.

This is still classical mechanics, and therefore completely deterministic. The reason why such a behavior is said to be chaotic is that any error in the determination of the trajectory will therefore be exponentially amplified over time. Thus a prediction becomes essentially impossible in practice, as in any practical (experimental) situation there are always errors. Chaos is therefore a feature of the unavoidable measurement errors rather than a problem coming from theory. Note that also Liouville's theorem of section 5.12 still holds for collections of trajectories. Thus, the density in phase space remains, for explicitly time-independent systems, constant, though the volume may become exponentially deformed.

This is quite different for quantum chaos, where quantum effects can introduce additional chaotic behavior, which leads too far beyond the scope of this lecture.

It is actually not necessary that a system shows the behavior (6.27) for all pairs of possible trajectories, i. e. initial conditions, nor for all times. It can well be that the system is chaotic for some cases of initial conditions, but not all. It is also possible that after some time of exponentially diverging trajectories come again close to each other. The simplest such system is actually a double pendulum. For small oscillations it shows no chaotic behavior, but as soon as the kinetic energy exceeds a critical value it becomes chaotic.

Classifying such features of a system is the purview of chaos theory. Interesting features of chaotic systems are, e. g., attractors. These are localized regions in phase space at which multiple trajectories, even from completely different initial conditions, coalesce, and stay there. If they do so without forming any kind of periodicity, the attractor is called strange. If the system is dissipative, and therefore the phase space density can change, the attractor can become a point in phase space, which is called a fixed point.

As many practically relevant systems, especially those of many degrees of freedom, can show chaotic behavior, this subject is of great importance. Due to its large number of phenomena and features, its detailed study warrants an own lecture, and it will not be continued here.

⁹There exists actually a mathematically more precise definition of what a chaotic system is, but for the present purpose this is sufficient.

6.5 The geometry of phase space

Classical mechanics has actually an interesting geometric interpretation, which warrants some thoughts. This is especially the case as geometric structures are prevalent in physics, and reappear in one way or another in all fundamental theories known.

This will become most evident when using phase space, and thus Hamiltonian mechanics. Note that phase space is always even-dimensional, with dimension $2n$ in the following. In such spaces there exist a particular group of matrices, the so-called symplectic matrices, $\text{Sp}(2n)$. These are the matrices A with the property

$$\begin{aligned} A^T J A &= J \\ J &= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \end{aligned} \quad (6.28)$$

where the elements of J are either zero matrices or (negative) unit matrices, each of dimension n . Note for further use that $J^{-1} = J^T = -J$ and $J^2 = -1$. It can be shown that for the submatrices of the matrix A

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

holds that

$$\begin{aligned} (a^T c)^T &= a^T c \\ (b^T d)^T &= b^T d \\ a^T d - c^T b &= 1. \end{aligned}$$

Furthermore, if $\lambda \neq 0$ is an eigenvalue of A , so is $1/\lambda$, λ^* and $1/\lambda^*$, where the last two can coincide with the first two if λ is real. Also, quite general statements about the multiplicities of eigenvalues can be made, which will not be needed here.

Consider now a not explicitly time-dependent Hamilton function H , and the two vectors

$$\begin{aligned} \vec{v} &= \begin{pmatrix} q_i \\ p_i \end{pmatrix} \\ \vec{\partial} &= \begin{pmatrix} \partial_{q_i} \\ \partial_{p_i} \end{pmatrix}, \end{aligned}$$

where the subvectors are n -dimensional, in phase space. Construct the vector

$$J \vec{\partial} H = \begin{pmatrix} \partial_{q_i} H \\ -\partial_{p_i} H \end{pmatrix}, \quad (6.29)$$

which contains Hamilton's equations. Especially, Hamilton's equation (5.11-5.12) take the compact form of a vector equation

$$\partial_t \vec{v} = J \vec{\partial} H.$$

Thus, the expression (6.29) describes the trajectory in phase space.

As a first example how this formulation could be advantageous, consider the total time derivative of H ,

$$d_t H = (\vec{\partial} H)^T \partial_t \vec{v} = (\vec{\partial} H)^T J \vec{\partial} H = 0.$$

Thus, the time-independence of the Hamilton function becomes now a geometric feature of phase space, as this hinged only on the features of the matrix J , rather than any other derivatives. It is a statement about the trajectories generated by the function H . This is quite similar in spirit to what the potential does - there it is a gradient in ordinary space which creates by Newton's equations the movement of the system. Here, the gradient of the Hamilton function in phase space, supplemented by the matrix J , creates by Hamilton's equation the movement, and the conservation of the Hamilton function along the trajectories is a geometric consequence of this.

Now, combine these insights with those of section 5.12. There it was shown that movement along a trajectory is created by the Hamilton function,

$$\begin{aligned} dq_i &= \frac{\partial H}{\partial p_i} dt \\ dp_i &= -\frac{\partial H}{\partial q_i} dt, \end{aligned}$$

which was actually a canonical transformation. This implies that a trajectory develops in phase space as

$$dv = J \vec{\partial} H dt.$$

In addition, any canonical transformation is given similarly by

$$dv = J \vec{\partial} G,$$

where the function G is the deviation of the generating function F_2 from the unity transformation, as defined in 5.12. As has been noted there, time evolution was anyhow only a special case of such a transformation. Thus, symplectic velocity fields $J \vec{\partial} G$ create all (infinitesimal) canonical transformations in phase space.

It is even possible to state more. Consider the matrix of derivatives of the canonical transformations

$$M = \begin{pmatrix} \frac{\partial q_i}{\partial Q_j} & \frac{\partial q_i}{\partial P_j} \\ \frac{\partial p_i}{\partial Q_j} & \frac{\partial p_i}{\partial P_j} \end{pmatrix}.$$

Because the canonical transformations are invertible, it follows that

$$M^{-1} = \begin{pmatrix} \frac{\partial Q_i}{\partial q_j} & \frac{\partial P_i}{\partial p_j} \\ \frac{\partial Q_i}{\partial q_j} & \frac{\partial P_i}{\partial p_j} \end{pmatrix}.$$

Add into this the relations (5.50-5.52). It then follows by explicit evaluation that

$$-JM = (JM^{-1})^T$$

holds. But this just defines a symplectic transformation, as this is equivalent to (6.28),

$$J = M^T J M.$$

Thus, a finite canonical transformation can be characterized by symplectic matrix. As a consequence, the scalar product

$$vw = v^T J w,$$

with v and w two vectors in phase space is invariant under any canonical transformations. A space endowed with such a metric is called a symplectic space or symplectic manifold.

Also the Poisson brackets can be integrated into this formulation,

$$\{F, G\} = -(\partial F)^T J (\partial G). \quad (6.30)$$

Thus, it is a scalar product in this symplectic space. Because such a scalar product is invariant under canonical transformations, as noted above, the invariance of Poisson brackets under canonical transformations, obtained in section 5.10, follows here trivially from the geometry of phase space. Especially,

$$\{v_i, w_j\} = -J_{ij}.$$

Therefore, the fundamental Poisson brackets (5.44-5.46) in fact define the metric of phase space.

This gives also the identification of the Poisson bracket as a differential operator in section 5.11 a geometric meaning. Since in (6.30) the expression $J\partial G$ defines a flow along a canonical transformation, the Poisson bracket acts as directional derivative with respect to the flow ∂F .

6.6 The relativistic string

In many areas of physics string-like objects appear. It is therefore useful to understand their classical behavior. To give this a further twist, it is interesting to consider a relativistic string.

For strings, the world line becomes a world sheet. As a consequence, at any fixed eigentime τ the string has an extension. This extension can be infinite or finite. In the latter case, the string can be closed, i. e., its ends are connected, or open. Here a finite string of length L will be considered.

Analogous to the eigentime then an eigenlength σ can be introduced. Both parameters together describe any point on the world sheet. The functions X_μ describing the position of the points of the world sheet in space-time are therefore functions of both parameters, $X_\mu = X_\mu(\sigma, \tau)$. Furthermore, as for the point particle of section 5.6.2, these functions should be reparametrization invariant

$$X^\mu(\sigma, \tau) = X^\mu(\sigma'(\sigma, \tau), \tau'(\sigma, \tau)) \quad (6.31)$$

such that the position of the world sheet is not depending on the parametrization.

Derivatives with respect to the two parameters will be counted by Latin indices a, \dots ,

$$\begin{aligned} \partial_{a,b,\dots} &= \partial_\tau, \partial_\sigma \\ \partial_0 &= \partial_\tau \\ \partial_1 &= \partial_\sigma. \end{aligned}$$

It is then possible to define the so-called induced metric on the world sheet as

$$h_{ab} = \partial_a X^\mu \partial_b X_\mu,$$

as a generalization of $h_{\tau\tau} = \dot{X}^\mu \dot{X}_\mu$, which had been used to define the action (5.19). Geometrically, $\sqrt{-\det h_{ab}} d\tau d\sigma$ is an infinitesimal element of the world sheet area.

The simplest possible Poincare-invariant action, which can be written down for this system, is the Nambu-Goto action

$$S_{NG} = \int_M d\tau d\sigma \mathcal{L}_{NG}$$

in which M is the world-sheet of the string and \mathcal{L}_{NG} is the Nambu-Goto Lagrangian

$$\mathcal{L}_{NG} = -\frac{1}{2\pi\alpha'} \sqrt{-\det h_{ab}} = -\frac{1}{2\pi\alpha'} \sqrt{\partial_\tau X_\mu \partial_\sigma X^\mu \partial_\sigma X_\rho \partial_\tau X^\rho - \partial_\tau X_\mu \partial_\tau X^\mu \partial_\sigma X_\rho \partial_\sigma X^\rho},$$

again the direct generalization of the point-particle action. In particular, the minimum area of the world sheet minimizes the action, analogously to the problem of minimizing the surface of a rotating object in section 5.1.2.

The constant α' is the so-called Regge slope. This Regge slope can be shown to be associated with the string tension T as $T = 1/(2\pi\alpha')$.

The Nambu-Goto action has two symmetries. One is invariance under reparametrization. This can be seen directly, as in the case of the point particle in section 5.6.2, except that now the Jacobian appears. The second invariance is Poincare invariance, which leaves the world-sheet parameters τ and σ invariant. However, the functions X_μ transform as

$$X'^\mu = \Lambda^\mu_\nu X^\nu + a^\mu$$

$$\partial_a \Lambda^\mu_\nu X^\nu \partial_b \Lambda^\gamma_\mu X_\gamma = \overbrace{\Lambda^\mu_\nu \Lambda^\gamma_\mu}^{\delta^\gamma_\nu} \partial_a X^\nu \partial_b X_\gamma = \partial_a X^\mu \partial_b X_\mu.$$

Thus, the induced metric is Poincare invariant, and hence also the action as well as the Lagrangian and any other quantity constructed from it is.

As in section 5.6.2 it is rather cumbersome to use an action involving a square root. To construct a simpler action, it is useful to introduce a world-sheet metric $\gamma_{ab}(\tau, \sigma)$. This metric is taken to have a Lorentz signature for some chosen coordinate system

$$\gamma_{ab} = \begin{pmatrix} + & 0 \\ 0 & - \end{pmatrix}.$$

Thus, this metric is traceless, and has a determinant smaller zero. With it the new action, the Brink-Di Vecchia-Howe-Deser-Zumino or Polyakov action,

$$S_P = -\frac{1}{4\pi\alpha'} \int_M d\tau d\sigma (-\gamma)^{\frac{1}{2}} \gamma^{ab} h_{ab} \quad (6.32)$$

is constructed, where γ denotes $\det \gamma_{ab}$.

As in case of the point particle, the world-sheet metric γ_{ab} has to have a non-trivial transformation property under reparameterizations,

$$\frac{\partial \omega'^c}{\partial \omega^a} \frac{\partial \omega'^d}{\partial \omega^b} \gamma'_{cd}(\tau', \sigma') = \gamma_{ab}(\tau, \sigma),$$

where the variables ω denote either σ and τ , depending on the index. This guarantees that for all invertible reparameterizations, which are continuous deformations of the identity transformation, the metric is still traceless and has negative determinant.

To obtain the relation of the Polyakov action to the Nambu-Goto action it is again necessary to obtain its equation of motion. This is most conveniently obtained using the variational principle. For this, the general relation for determinants of metrics

$$\delta \gamma = \gamma \gamma^{ab} \delta \gamma_{ab} = -\gamma \gamma_{ab} \delta \gamma^{ab}$$

is quite useful.

Abbreviating the Polyakov Lagrangian by L_P and performing a variation with respect to γ yields

$$\begin{aligned}\delta S_P &= -\frac{1}{4\pi\alpha'} \int d\tau d\sigma \left(L_P - (-\gamma - \delta\gamma)^{\frac{1}{2}} (\gamma^{ab} + \delta\gamma^{ab}) h_{ab} \right) \\ &= -\frac{1}{4\pi\alpha'} \int d\tau d\sigma \left(L_P - (-\gamma + \gamma\gamma^{cd}\delta\gamma_{cd})^{\frac{1}{2}} (\gamma^{ab} + \delta\gamma^{ab}) h_{ab} \right) \\ &= -\frac{1}{4\pi\alpha'} \int d\tau d\sigma \left(L_P - (-\gamma)^{\frac{1}{2}} (1 - \gamma^{cd}\delta\gamma_{cd})^{\frac{1}{2}} (\gamma^{ab} + \delta\gamma^{ab}) h_{ab} \right).\end{aligned}$$

Expanding the term with indices cd up to first order in the variation leads to

$$\begin{aligned}\delta S_P &= -\frac{1}{4\pi\alpha'} \int d\tau d\sigma \left(L_P - (-\gamma)^{\frac{1}{2}} \left(1 - \frac{1}{2}\gamma^{cd}\delta\gamma_{cd} \right) (\gamma^{ab} + \delta\gamma^{ab}) h_{ab} \right) \\ &= -\frac{1}{4\pi\alpha'} \int d\tau d\sigma \left(L_P - (-\gamma)^{\frac{1}{2}} \left(\gamma^{ab} + \delta\gamma^{ab} - \frac{1}{2}\gamma^{cd}\gamma^{ab}\delta\gamma_{cd} \right) h_{ab} \right).\end{aligned}$$

The second term is again the Polyakov Lagrangian, canceling the zero-order term. Then only

$$\delta S_P = -\frac{1}{4\pi\alpha'} \int d\tau d\sigma (-\gamma)^{\frac{1}{2}} \left(h_{ab} - \frac{1}{2}\gamma_{ab}\gamma_{cd}h^{cd} \right) \delta\gamma^{ab}$$

is left.

The condition that this expression should vanish yields the equation of motion for the world-sheet metric as

$$h_{ab} = \frac{1}{2}\gamma_{ab}\gamma_{cd}h^{cd} \quad (6.33)$$

Division of each side by its determinant finally yields

$$\begin{aligned}\frac{h_{ab}}{(-h)^{\frac{1}{2}}} &= \frac{1}{2} \frac{\gamma_{ab}(\gamma_{cd}h^{cd})}{\left(\det -\frac{1}{2}\gamma_{ab}\gamma_{cd}h^{cd}\right)^{\frac{1}{2}}} \\ &= \frac{1}{2} \frac{\gamma_{ab}(\gamma_{cd}h^{cd})}{\left(\left(\frac{1}{2}\gamma_{cd}h^{cd}\right)^2 \det -\gamma_{ab}\right)^{\frac{1}{2}}} \\ &= \frac{\gamma_{ab}}{(-\gamma)^{\frac{1}{2}}}\end{aligned}$$

In the second line it has been used that $\gamma_{cd}h^{cd}$ is a scalar, permitting it to pull it out of the determinant. The result implies that h and γ are essentially proportional.

Inserting this result in the Polyakov action yields

$$S_P = -\frac{1}{4\pi\alpha'} \int d\tau d\sigma \gamma^{ab}\gamma_{ab}(-h)^{\frac{1}{2}} = -\frac{1}{2\pi\alpha'} \int d\tau d\sigma (-h)^{\frac{1}{2}} = S_{NG}$$

showing that it is indeed equivalent to the Nambu-Goto action, where the fact that the quantity $\gamma^{ab}\gamma_{ab}$ is two, due to the Lorentz signature of γ , has been used.

The Polyakov action thus retains the Poincare and reparametrization invariance of the Nambu-Goto action. The Poincare invariance follows since γ is Poincare invariant, since it is proportional to the Poincare-invariant induced metric, thus

$$\gamma^{ab'} = \Lambda \gamma^{ab} = \gamma^{ab}.$$

The diffeomorphism invariance follows directly from the transformation properties of the world-sheet metric, in total analogy with the point-particle case, but considerably more lengthy since track of both variables has to be kept.

The redundancy introduced with the additional degree of freedom γ grants a further symmetry. This is the so-called Weyl symmetry, given by

$$\begin{aligned} X'^\mu(\tau, \sigma) &= X^\mu(\tau, \sigma) \\ h'_{ab} &= h_{ab} \\ \gamma'_{ab} &= e^{2\omega(\tau, \sigma)} \gamma_{ab}. \end{aligned}$$

for arbitrary functions $\omega(\tau, \sigma)$. The origin of this symmetry comes from the unfixed proportionality of induced metric and the world-sheet metric. The expression of γ in terms of the induced metric h is invariant under this transformation,

$$\frac{\gamma'_{ab}}{(-\gamma')^{\frac{1}{2}}} = \frac{\gamma_{ab} e^{2\omega}}{(-\gamma')^{\frac{1}{2}}} = \frac{\gamma_{ab} e^{2\omega}}{(-\gamma e^{4\omega})^{\frac{1}{2}}} = \frac{\gamma_{ab}}{(-\gamma)^{\frac{1}{2}}}.$$

Also the action is invariant. To see this note that γ_{ab} is indeed a metric. Since $\gamma_{ab}\gamma^{ab}$ has to be a constant, as noted before, this implies that

$$\gamma'^{ab} = e^{-2\omega} \gamma^{ab}.$$

As a consequence, the expression appearing in the action transforms as

$$(-\gamma')^{\frac{1}{2}} \gamma'^{ab} = (-\gamma e^{4\omega})^{\frac{1}{2}} \gamma^{ab} e^{-2\omega} = (-\gamma)^{\frac{1}{2}} \gamma^{ab}.$$

Thus, the Weyl invariance is indeed a symmetry.

6.7 First-order and second-order constraints

It is not always possible to formulate constraints quite as concise as wished for. Consider the not explicitly time-dependent situation. In particular, given a constraint $f = 0$, it should remain a constraint over time,

$$\frac{df}{dt} = 0. \tag{6.34}$$

The time evolution is governed by (5.43), as this can be taken to be a postulate, and thus

$$\{f, H\} = g, \quad (6.35)$$

with g some function. If f should be a constraint this requires g to be zero, $g = 0$, as otherwise (6.34) is violated. Of course, this may entail another constraint from $\{g, H\}$. Constraints for which the Poisson bracket with the Hamilton function identically vanish, but cannot be written as the Poisson bracket of the Hamilton function with some other quantity are called primary constraints. All other constraints, such as g , are called secondary constraints, provided these are not linearly dependent on the primary constraints. All of them have to hold. Note that secondary constraints can only be defined once the Hamilton function is known.

It is possible to reclassify the set of primary and secondary constraints. Given the total sets of constraints ϕ_i , constraints of the first kind γ_i are the subsets of constraints which fulfill

$$\{\gamma_i, \phi_i\} = 0,$$

for all other constraints. All constraints which are not of the first kind are called of second kind, χ_i , thus

$$\{\phi_i\} = \{\gamma_i\} \cup \{\chi_i\}.$$

This implies there exists functions C_{ij} with

$$\{\chi_i, \chi_j\} = C_{ij}$$

which form an antisymmetric matrix C .

If the matrix C is invertible, define the Dirac brackets as

$$\{F, G\}_D = \{F, G\} - \{F, \chi_i\}(C^{-1})_{ij}\{\chi_j, G\}.$$

By construction the Dirac brackets of all constraints of the first kind still vanish. Furthermore

$$\{\chi_i, \chi_j\}_D = \{\chi_i, \chi_j\} - C_{ik}(C^{-1})_{kl}C_{lj} = C_{ij} - C_{ij} = 0.$$

Therefore now all brackets between constraints vanish, and all constraints act on equal footing. Because of (6.35) the Dirac brackets of all constraints with the Hamilton function also vanish. Therefore the time-evolution formulated in terms of the Dirac brackets still respect the constraints.

Without proof, it can be shown that now all appearances of the Poisson brackets can be replaced by Dirac brackets, and therefore everything remains form-invariant. The advantage is that with respect to the Dirac bracket all constraints are always exactly

fulfilled, and there is no non-trivial time evolution which needs to be fulfilled. In this way all constraints are satisfied identically. In terms of the Poisson brackets, constraints of the second kind are only fulfilled if evaluated on the solutions of the equations of motions.

In classical physics, this is irrelevant, as anyhow only solutions to the equations of motions are searched for. In the context of quantum physics this difference becomes relevant: In quantum physics also trajectories which do not fulfill the equations of motions play a role, and therefore primary and secondary constraints would make a difference. Therefore, in the context of constrained quantum physics a clean formulation uses the Dirac brackets rather than the Poisson brackets.

To see how brackets can play a role for quantum physics, it is useful to have a little preview to see how quantum physics could have something to do with the Hamilton function.

6.8 A preview of quantum physics

This lecture fully reviews classical mechanics. Except for specifying the Hamilton or Lagrange functions for a given system, all knowledge on mechanics is encoded in the presented formalism. This by no means guarantees that all mechanical problems are solved. For many systems the arising equations of motions are so involved that an exact solution is not possible. Even approximate or numerical solutions can pose serious challenges. In fact, in contrast to the case of ordinary differential equations the mathematical foundation of partial differential equations is much less developed. It is therefore even possible that even the existence of a solution is a non-trivial question. The problem of fluids is a famous and notorious example. Furthermore, it may be far from trivial, especially for complex systems with many degrees of freedom, to write down a consistent Hamilton or Lagrange function, as it is not easy to find an adequate, say, potential for a given observed system. In the limit of very large numbers of degrees of freedom, this leads to classical statistical mechanics, and ultimately classical thermodynamics. Nonetheless, these are from a mechanical point of view nothing conceptually new, though introducing physically new concepts.

Leaving aside all the involved technical problems, classical mechanical systems are therefore fully formulated. A conceptually new situation arises only when introducing quantization, and quantum physics. In fact, a whole new set of postulates will be necessary to do so. It is the necessity of new postulates which sets quantum mechanics apart, and makes it something conceptually new. It will be the contents of the corresponding lectures to deal with these postulates in detail.

However, it is still a quite interesting question of how classical physics can be considered

as being part of something larger, which gives a preview of what comes. This will be done here. It also gives some more insights into various concepts in classical mechanics.

Start with a conservative system with the Hamilton function

$$H = T + V = E,$$

where E is the total energy. Following section 5.13, it is then possible to find a canonical transformation

$$F_2(q, P, t) = W(q, P) - Et$$

such that $h = 0$, i. e. a solution to the Hamilton-Jacobi equation. Thus, P and Q in these new coordinates are constant. Since, according to section 5.13.3, the function W is related to the action, this has an interesting implication. The function W only depends on the variables q as the P are constant, by construction. The condition that $W(q, P)$ should be constant therefore defines surfaces of constant action in the configuration space. The function F_2 , however, changes with time, but in a linear fashion. Thus, the requirement that F_2 should be constant defines how the system moves, as a function of time crossing equal-action surfaces in configuration space. In a sense, the system moves like waves over constant action surfaces, and forms action waves.

This is quite abstract, and it is therefore important to understand what this means. This is best understood by first simplifying the problem to a single particle, using the ordinary space coordinates for the description.

Consider first the speed of the action waves, i. e. what is the rate of change of the action $S = F_2$ when moving during some infinitesimally time to some point. This is given by the differential of¹⁰ S ,

$$dS = \partial_t S dt + \frac{\partial S}{\partial x_i} dx_i = -E dt + d\vec{r} \vec{\partial}_i W = -E dt + \vec{u} \vec{\partial} W dt.$$

where the wave speed is defined as $\vec{u} = d\vec{r}/dt$.

If the system should stay at constant action this requires

$$\vec{u} \vec{\partial} W = E.$$

Since $\vec{\partial}_i W$ is perpendicular, by construction, to the surfaces of constant action. Since W is part of a canonical transformation function F_2 , this furthermore implies for ordinary coordinates

$$\vec{p} = \vec{\partial} W$$

¹⁰The notation $\vec{\partial} f$ is a vector with components $\partial f / \partial x_i$.

Thus, the particle moves also perpendicular to the surfaces of constant action. Thus, the motion of the particle is in the same direction as the action waves: Particles essentially ride action waves. Especially, for the free particle

$$|\vec{u}| = \frac{|E|}{|\vec{\partial}W|} = \frac{|E|}{|\vec{p}|} = \frac{|E|}{m|\vec{v}|}$$

Since the ratio $|E|/m$ is fixed this implies that the relative direction of \vec{u} and \vec{v} are also fixed and in fact they are inverse proportional. This has an interesting interpretation, though it is not obvious that it is true in general: Movement of particles can be equivalently described by either the movement as a trajectory in some suitable space or as action waves. This already hints at a kind of duality between waves and particles, which plays an important role in quantum physics. One major difference will be, however, that there is not yet any quantum in the description: Both energy and momentum can take any arbitrary, continuous value. The major change induced by quantum physics will be that this is no longer possible, and often only discrete, i. e. quantized, values will be possible.

To further the transition, it is useful to rewrite the equations of mechanics a little bit more to make the duality more apparent. For this, compare the Hamilton-Jacobi equation with the magnitude of the wave speed,

$$\begin{aligned} u &= \frac{|E|}{p} = \frac{|E|}{\sqrt{2m(E-V)}} \\ E &= \frac{1}{2m} \left((\vec{\partial}W)^2 \right) + V. \end{aligned}$$

Since furthermore $\vec{\partial}F_2 = \vec{W}$ and since $F_2 = S$ the action, according to section 5.13.3, this leads to

$$\left(\vec{\partial}S \right)^2 = \frac{1}{u^2} (\partial_t S)^2 \quad (6.36)$$

which can be considered as the wave-equation for classical mechanics.

While classical systems adhere to it, this equation is no longer valid at quantum scales. It is here where the postulates of quantum physics set in, by replacing (6.36) by a new equation, the Schrödinger equation, which in the long-distance limit reduces to (6.36). It turns out that in the end a reformulation of (6.36) using the Hamilton function is better suited for the postulates necessary, but this will actually be a minor detail. More important is that the postulates will require to also replace the concept of trajectories and measurements, and therefore the mathematical foundation, of classical mechanics. But still, at long distances, it will come back to (6.36).