Classical Mechanics

Draft

Heribert Weigert
heribert.weigert@uct.ac.za
typeset with LaTeX on July 31, 2020, 13:17

Contents

Contents ii

Preliminaries . . . vi

1 Elementary Newtonian Mechanics 1

1.1 Newton's laws . . . 1
1.2 Inertial frames and Galilei transformations . . . 5
1.3 Mathematical interlude: matrix Lie groups . . . 9
1.3.1 Matrix Lie groups with applications in classical and quantum mechanics . . . 9
1.3.2 Parametrizing the Lie algebras of unitary and orthogonal groups, dimensions . . . 16
1.3.3 Orthogonal and unitary Lie-groups and algebras, a summary . . . 18
1.3.4 Special properties of SU(2) and SO(3) . . . 18
1.4 The Galilei group – the complete set of transformations that relates any two inertial frames in non-relativistic mechanics . . . 21
1.5 Arbitrary frames including non-inertial frames, fictitious forces . . . 23
1.6 Simple mechanical systems – definitions of crucial concepts . . . 25
1.6.1 Closed and open systems and the center of mass principle . . . 25
1.6.2 Work and energy . . . 27
1.6.3 Central potentials and angular momentum conservation . . . 30
1.6.4 Closed systems and their conservation laws . . . 31
1.7 Degrees of freedom, configuration space, and phase space . . . 32
1.8 Configuration and phase space at work – examples . . . 33
1.8.1 Example: The harmonic oscillator . . . 33
1.8.2 Example: The damped harmonic oscillator – an open system . . . 36
1.8.3 Example: the pendulum, spherical and planar, mathematical and physical . . . 41
1.9 Existence and uniqueness of solutions, local flow in phase space . . . 44
1.10 Linear systems and linear approximations . . . 45
1.10.1 The forced harmonic oscillator . . . 46
1.11 Coupled oscillators . . . 52
1.11.1 Linear chains . . . 54

2 From Newton to Lagrange – systems with constraints 79

2.1 Degrees of freedom and constraints . . . 79
2.2 d'Alembert's principle and the derivation of Lagrange's equation . . . 84
2.3 Variational principles and the Euler Lagrange equations . . . 91
2.3.1 D'Alembert's principle as a variational principle . . . 91
2.3.2 Elements of variational calculus . . . 92
2.3.3 Hamilton's variational principle . . . 96
2.3.4 Reconstructing the forces of constraint after the fact . . . 98
2.3.5 Non-uniqueness of the Lagrangian . . . 99
2.3.5.1 Gauge transformations of the Lagrangian . . . 99
2.3.5.2 Admissible transformations of the generalized coordinates . . . 101

3 Applications 104

3.1 Kepler's problem . . . 104
3.1.1 Foucault's pendulum, or "how to prove quantiatively that the earth is rotating witout resorting to astronomy" . . . 109
3.2 Rigid bodies, spinning tops . . . 112

4 The Hamiltonian description of classical mechanics **113**
4.1 Towards a phase space description with generalized coordinates . . . 113
4.2 Canonical systems . . . 116

5 Symmetries and conservation laws – Noether's theorem **118**
5.1 Motivation . . . 118
5.2 Noether's theorem . . . 119
5.3 Extending Noether's theorem . . . 122

6 Elements of mechanics in its phase space formulation **124**
6.1 The general symplectic structure of the canonical equations . . . 124
6.2 Preservation of the phase space volumes under time evolution . . . 129
6.3 Poisson brackets as a realization of the symplectic bilinear form for phase space gradients . . . 131

7 Outlook – there is more to classical mechanics **135**

A Symmetries on phase space **136**
A.1 Generalizing the Galilei group to phase space . . . 136
A.2 The $\mathsf{O}(4)$ symmetry of the Kepler problem . . . 136

B Mathematical aside – $\mathfrak{C}$ and $T\mathfrak{C}$: configuration space and phase space as mathematical objects **137**
B.1 Concepts . . . 137
B.1.1 Manifolds and sub-manifolds . . . 137
B.1.2 Analysis with constraints – tangent bundles and the like . . . 140

C Symplectic manifolds **141**
C.1 Gathering input . . . 141
C.1.1 A quick characterization from stackexchange . . . 141
C.1.2 Candidates for literature . . . 141
C.2 Solving Kepler via quaternions – a little math excursion . . . 143
C.3 Applications of elliptic functions . . . 144

Bibliography **145**

The following todo list contains orange items which are short questions to the reader. Should you see any red items they are reminders to the author to iprove the text.

Todo list

Why not one but the other? . . . 7

Check that this is indeed the case. . . . 11

Verify this for $n = 2, 3$. . . . 13

Assume that $\alpha(t) = \frac{1}{2}\boldsymbol{a}t^2$. What is the relative acceleration of the frames? What is the fictitious force in frame B. (Assume that the particle is moving inertially in frame A.) . . . 23

Verify this for yourself! . . . 24

Generalize this to the case of accelerated rotation, where $R(t) = e^{(\hat{\omega}^a i t^a)\omega(t)}$. . . . 24

Derive that $\boldsymbol{F}(\boldsymbol{r}) = -\boldsymbol{\nabla}U(\boldsymbol{r})$ by taking the time derivative in (1.6.20) . . . 28

fix this and explain . . . 35

Fix Graphics . . . 35

physical and mathematical pendulum, constraints, tension of rod . . . 41

Fix Graphics . . . 42

Fix Graphics . . . 43

Why? . . . 45

under construction . . . 52

that's probably too much – should probably insert some discussion about widening Gaussians . . . 73

Fix Graphics . . . 82

Fix Graphics . . . 82

Fix Graphics . . . 89

Fix graphics . . . 93

need to do this in 3d . . . 96

Verify this claim! . . . 98

This needs examples!! The mathematical pendulum would be a good one. . . . 98

Fix graphics . . . 101

finish Foucault approx . . . 110

Finish this example! . . . 125

Move generating functions here . . . 127

Check that this is linear in both slots. . . . 128

Fix graphics 131
Fix graphics 3 times 131
Fill in 133
Work this out explicitly 133
Fix Graphics 137
Fix Graphics 137
Fix Graphics 138

Preliminaries

Organizational matters

- Course split into two parts Classical Mechanics (Assoc. Prof. Heribert Weigert) and Quantum Mechanics (Assoc. Prof. Roger W. Fearick)
- Class representative (elect) and coordinate time for 3hours of tutorials per week with class tutor (Max Richter) [by Tuesday]

Textbooks

- Scheck: "Mechanics: From Newton's Laws to Deterministic Chaos" chapters 1 & 2. [1]

  This is a quite modern treatment. In its later chapters it steps far beyond the material covered in this course
- Kibble and Berkshire "Classical Mechanics (5th Edition)", the first few chapters [2]

  Similar in level to Scheck, slightly different style. Nice list of problems.
- Morin: "Introduction to CLASSICAL MECHANICS with problems and solutions".

  A standard modern textbook. Good training in practicalities. Supporting arguments often avoided. This will not do as a main source of material.
- Jose & Saletan: "Classical dynamics. A conteporary approach"

  Modern, with a slight leaning towards differntial manifolds in a pedestrian sort of way.
- Goldstein: "Classical Mechanics" (2nd and 3rd edition) [3]
  The classic classical mechanics textbook for a long time in the west. Still one of the most complete descriptions.
- Greiner: "Systems of particles and Hamiltonian mechanics"
  Relatively modern text – Valuable resource even if you do not like the explanations: the books of Greiner's series have most calculational steps *explicitly* worked out.
- Landau & Lifshitz: "Mechanics" (3rd edition)

  A classic, concise, the counterpart to Goldstein's book in the east, very illuminating for the advanced student.
- Schaum's outline series: Theoretical Mechanics

Overview: Classical Mechanics in 2nd year

- Elementary Newtonian Mechanics
  - Newton's Laws (1687) and their interpretation
  - Uniform rectilinear motion and inertial systems
  - Inertial frames in relative Motion
  - Momentum and force
  - Space, time, and forces
  - The two-body system with internal forces, center-of-mass and relative motion. Example: the gravitational force (Kepler's Problem), center-of-mass and relative momentum
  - Systems of finitely many particles
  - Conservation laws: center-of-mass motion, momentum and angular-momentum conservation, energy conservation
  - Closed n-particle systems
  - Galilei transformations, space and time with Galilei invariance
  - Conservative force fields
  - One-dimensional motion of a point particle: the harmonic Oscillator, the planar mathematical Pendulum
  - *Phase space* for the n-Particle System (in $\mathbb{R}^3$)
  - Solving equations of motion $\dot{x} = F(x,t)$ (existence and uniqueness physical consequences thereof), linear homogeneous and inhomogeneous systems.
  - Non-inertial frames, prime example: rotating reference systems: Coriolis and centrifugal forces
  - Scattering of two particles that interact via a central force (example Coulomb scattering)
  - Mechanical bodies of finite extension
- The Principles of Canonical Mechanics
  - Constraints and generalized coordinates (bodies of finite extensions: relative spatial relations of the atoms in the body are fixed; particles moving on prescribed trajectories (roller coasters of sorts))
  - The core of canonical mechanics: *variational calculus* as a means to obtain equations of motion from an underlying function(al):
    - D'Alembert's Principle
    - Virtual Displacements
    - Lagrange's Equations
    - Variational Principles
    - Hamilton's Variational Principle(1834)

All in on to one relation to symmetries of the problem, see Noether

List all symmetries and ways to get from one inertial frame to another

Aside from practical applications: To reinforce what inertial frames really are and how much of an abstraction they represent.

How to count degrees of freedom for real and eliminate "fluff" coordinates.

The mathematical underpinnings of canonical mechanics, rephrasing Newtons laws in a more powerful manner: One function contains *all* information.

- The Euler–Lagrange Equations and the *Lagrangian function*
  - Non-uniqueness of the Lagrangian function (gauge transformations of the Lagrangian function)
  - Choice of coordinates: Admissible transformations of the generalized coordinates
- The *Hamiltonian function* and its relation to the Lagrangian function, Legendre transformations for one and several variables.
- Canonical systems
- The variational principle in the context of Hamiltonian functions
- From symmetries to conservation laws: *Noether's Theorem* – translations and rotations
- Powerful mathematical tools of classical mechanics:
  - Canonical transformations, examples, structure
  - The symplectic structure of phase space, Liouville's theorem, Poisson Brackets
  - Integrals of motion

› ... and if, inexplicably, there is enough time:

- Hamilton–Jacobi theory, integrable systems, angle and action variables

Modern field theory uses exactly the same tool set.

The Hamiltonian (function) setting is a convenient starting point to develop quantum mechanics.

Systems that allow a full variational treatment, can be described by a Lagrangian and Hamiltonian.

1 Elementary Newtonian Mechanics

1.1 Newton's laws

> From wikipedia (*much more there*): **Sir Isaac Newton** PRS MP (25 December 1642 – 20 March 1727 (Julian) [Gregorian: 4 January 1643 – 31 March 1727]) was an English physicist, mathematician, astronomer, natural philosopher, alchemist and theologian, who has been "considered by many to be the greatest and most influential scientist who ever lived." His monograph Philosophiae Naturalis Principia Mathematica, published in 1687, lays the foundations for most of classical mechanics. Newton showed that the motions of objects on Earth and of celestial bodies are governed by the same set of natural laws, by demonstrating the consistency between Kepler's laws of planetary motion and his theory of gravitation, thus removing the last doubts about heliocentrism and advancing the Scientific Revolution.



Newton's laws (1687) may be considered the foundation of physics. Historically for the first time we see the combination of mathematical abstraction linked to experimental observation that are the hallmark of physics until today.

Only slightly paraphrasing the original, they are

I. Every body continues in its state of rest or of uniform rectilinear motion, except if it is compelled by forces acting on it to change that state.

II. The change of motion is proportional to the applied force and takes place in the direction of the straight line along which that force acts.

III. To every action there is always an equal and contrary reaction; or, the mutual actions of any two bodies are always equal and oppositely directed along the same straight line.

What do they imply? Any takers?

Despite the paraphrasing you note that the language is still somewhat archaic. The language is more colloquial than scientific, concepts like the *state of motion*, *uniform rectilinear motion*, and what a *force* might be remain unexplained. Many of the notions we take for granted in a more modern description like the idea of inertial frames and force vectors do not appear at all, indeed some of these concepts had not been formulated or assigned the sharp definitions we associate them with today.

I will now turn to a more modern formulation and introduce notions and concepts that help to provide the necessary amount of precision. We owe it to Descartes that we have grown used to specifing locations in space using coordinate systems, and we readily use Cartesian coordinates to do so. Such coordinate systems are called *frames*. Frames introduce the notion of a coordinate origin into space, which is an act of choice in our description of space, not a feature of space itself as will be discussed in more detail below. The literature often uses the notion of an observer to essentially make the same statement: the location of that imaginary observer marks the origin of a specific coordinate system, nothing more, nothing less.

Newtons first law makes an existence statement about a special type of frame:

I. **Inertial frames**: In nature, there exist *inertial frames* in which the trajectory $\boldsymbol{r}(t)$ of every object, in the absence of a force, satisfies $\ddot{\boldsymbol{r}} = 0$.

- The state of motion of an object (a body) refers to its trajectory $\boldsymbol{r}(t)$ in three dimensional Euclidean space $\mathbb{E}^3$, which is just $\mathbb{R}^3$ together with the scalar product $\langle \boldsymbol{a}, \boldsymbol{b} \rangle := a_i b_i$ (summation convention). The latter gives us a means to measure length and angles in the conventional way.

- $\mathbb{E}^3$ as defined above is simply a Euclidean metric space.

  This is slightly inaccurate: the physical configuration space has no preferred points. In particular there is no preferred origin $\mathbf{0}$ (the neutral element under vector addition), which is an essential ingredient in the make up of a vector space: only relative distances matter.

  - Another way of saying this is that physical space is *translationally invariant* or *homogeneous*: In empty space there is no preferred location. If one translates (moves) the whole system under consideration (or the observer or) by some fixed vector distance $\boldsymbol{a}$ the system behaves "the same" in the sense that the relative distance vectors (say $\boldsymbol{r}_i - \boldsymbol{r}_j$ for the locations of a pair of bodies labelled i and j respectively) of the moving bodies remain the same at all times as at the original location.
    Note that this is what mathematicians call an affine space, $\mathbb{E}^3$ is the vector space underlying this physical affine space.
  - This is complemented by *rotation invariance* or *isotropy*: In empty space, there is no preferred direction. It does not matter if we rotate space (or the observer), the relative motion of the system's constitutents remain unaffected.

- In practice, we define trajectories $\boldsymbol{r}(t)$ with respect to an observer, say at $\boldsymbol{o}(t)$ and introduce some type of coordinate system from the perspective of the observer, a *frame*.

  The choice of a coordinate system fixes both an origin and an orientation, thus it apparently breaks translational and rotational symmetry in how we view physical space: The underlying symmetry of space is hidden in our freedom to choose different frames in which we observe the same physical events.

- The equation

$$\frac{d^2}{dt^2}\boldsymbol{r} =: \ddot{\boldsymbol{r}} = 0 \tag{1.1.1}$$

  encodes the idea of uniform rectilinear motion: a state of motion with constant velocity and therefore vanishing acceleration,

  In an given *inertial frame* when forces are absent the equation of motion $\ddot{\boldsymbol{r}} = 0$ is easily solved: There are two (vectorial) integration constants $\boldsymbol{r}_0$ and $\boldsymbol{v}_0$ that parametrize the trajectory:

$$\boldsymbol{r}(t) = \boldsymbol{r}_0 + \boldsymbol{v}_0 t \tag{1.1.2}$$

  where t is time.

This is quite the abstraction: there is no space free of gravitational force on earth!

- Given this definition, we note that the first law makes an both an existence claim and provides a definition for inertial frames.

  Viewed this way this is indeed more than just a special case of the second law with $\boldsymbol{F} = 0$.

Imagine yourself jumping from the 10m platform of a diving tower and watching the diving pool accelerate towards you.

- Not all frames are inertial: Imagine an accelerated observer and his (her, for political correctness) *rest frame* (the frame he carries with him, which in this case is accelerated with him). To such an observer any other object will appear to accelerate, even if no force is acting on the object.

This assumption is no longer correct at relativistic speeds, the correct treatment leads to special relativity.

- *Time* plays a special role in all this: It is tacitly assumed that time differences measured by any

observer (in any frame) is the same. Formally, in two frames A and B we require that both observers are using the same units to measure time and that

$$(t_1^A - t_2^A)^2 \stackrel{!}{=} (t_1^B - t_2^B)^2 \tag{1.1.3}$$

This is to say that time is a one dimensional real vector space, endowed with a length measurement and translational invariance, a one dimensional affine space. The most general transformation that respects the vector space nature of this space are one dimensional linear maps (multiplications with real numbers $\lambda^{BA} \in \mathbb{R}$ (specific to the two frames A and B):

$$t_i^B = \lambda^{BA} t_i^A \tag{1.1.4}$$

If these are to respect Eq. (1.1.3) we find that

$$(t_1^B - t_2^B)^2 = (\lambda^{BA})^2 (t_1^A - t_2^A)^2 \stackrel{!}{=} (t_1^A - t_2^A)^2$$

i.e. that $\lambda^{BA} = \pm 1$. $\lambda^{AB} = -1$ constitutes a reversal of the time arrow (backward running clocks). To allow this is to state that physical systems have time reversal invariance. This is indeed the case for all closed physical systems and the reason we have required $(t_1^A - t_2^A)^2 \stackrel{!}{=} (t_1^B - t_2^B)^2$ instead of $(t_1^A - t_2^A) \stackrel{!}{=} (t_1^B - t_2^B)$.
For non-closed systems (systems with friction for example) time reversal invariance is absent, energy dissipates into the environment (as heat, in the case of friction), and can not be recovered.
In addition to time reversal, time translations by constant time offsets β

$$t_i^B = t_i^A + \beta^{BA} \tag{1.1.5}$$

are allowed by Eq. (1.1.3) since β^{BA} drops from time differences:

$$(t_1^B - t_2^B)^2 = ((t_1^A + \beta^{BA}) - (t_2^A + \beta^{BA}))^2 \stackrel{\text{automatically}}{=} (t_1^A - t_2^A)^2$$

Combining (1.1.4) and (1.1.6) leads us to the full set of inhomogeneous transformations between the time coordinates of two frames A and B

$$t_i^B = \lambda^{BA} t_i^A + \beta^{BA} \tag{1.1.6}$$

This is what remains of rotational invariance in a one dimensional system *after choosing units* for our length measurement.
Had we not chosen units $\lambda^{AB} \in \mathbb{R}$ would be arbitrary.

Reminder 1.1 – canonical scalar products on $\mathbb{R}^n$:
The canonical scalar product in $\mathbb{R}^n$ is given by

$$\begin{aligned} \langle , \rangle : \mathbb{R}^n \times \mathbb{R}^n &\to \mathbb{R} \\ (\boldsymbol{u}, \boldsymbol{v}) &\mapsto \langle \boldsymbol{u}, \boldsymbol{v} \rangle := \boldsymbol{u}^t \cdot \boldsymbol{v} \end{aligned} \tag{1.1.7}$$

This is positive definite ($\langle \boldsymbol{u}, \boldsymbol{u} \rangle > 0$ for all $\boldsymbol{u} \in \mathbb{R}^n \setminus \{\boldsymbol{0}\}$) and bilinear (linear in both the first $[\langle \alpha \boldsymbol{u} + \beta \boldsymbol{v}, \boldsymbol{w} \rangle = \alpha \langle \boldsymbol{u}, \boldsymbol{w} \rangle + \beta \langle \boldsymbol{v}, \boldsymbol{w} \rangle]$ and second components $[\langle \boldsymbol{u}, \alpha \boldsymbol{v} + \beta \boldsymbol{w} \rangle = \alpha \langle \boldsymbol{u}, \boldsymbol{v} \rangle + \beta \langle \boldsymbol{u} \boldsymbol{w} \rangle]$ for all $\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \in \mathbb{R}^n$ and $\alpha, \beta \in \mathbb{R}$).

II. $\dot{\boldsymbol{p}} = \boldsymbol{F}$: The change of momentum (motion) of any *object* (or body) is equal to the force applied to its *center of mass*.

- Here we have already assumed that a force $\boldsymbol{F}$ ($\in \mathbb{R}^3$, units of $\frac{\text{mass}\cdot\text{length}}{\text{time}^2}$ suppressed) is vectorial in nature
- Here we have interpreted *motion* to refer to the momentum $\boldsymbol{p}(t)$ of the object along its trajectory and write the equation of motion as

$$\dot{\boldsymbol{p}} = \boldsymbol{F} \tag{1.1.8}$$

This definition avoids talking about mass.

- In a second step one can relate momentum to velocity

$$\boldsymbol{p}(t) := \frac{d}{dt}(m\boldsymbol{r})(t) \tag{1.1.9}$$

As opposed to the gravitational mass or weight of the particle

The factor of proportionality m introduced here is the *inertial mass* of the particle.

Both, Eq. (1.1.8) and Eq. (1.1.9), are part of the interpretation of Newton's second law, although this is not spelled out directly in the original formulation.
If the mass of the object is constant in time, the equation of motion Eq. (1.1.8) becomes

$$m\ddot{\boldsymbol{x}} = \boldsymbol{F} \tag{1.1.10}$$

Note that this is *not* correct for a rocket under thrust, in which the mass changes drastically with time, requiring to add a term $\dot{m}\boldsymbol{v}_{\text{exhaust}}$ to the left hand side where generically $\dot{m} < 0$.

- Eq. (1.1.10) implicitly assumes either point particles or that the force acts on the *center of mass* of an extended object.
  For much of this course we will think of the mechanics of point particles to get our bearings. A proper discussion of rigid bodies will be attempted in Sec.???

Aside 1.1 – relativistic corrections:

Newtons second law in the form presented here, in particular Eqns. (1.1.9), and(1.1.10), is only a good description of reality as long as the velocities are much smaller than the speed of light, i.e. if $\frac{\dot{r}}{c} \ll 1$.

If this is not the case Eq. (1.1.9) is replaced by the relativistic expression

$$\boldsymbol{p}(t) := \frac{1}{\sqrt{1-\frac{\dot{\boldsymbol{r}}^2}{c^2}}}\frac{d}{dt}(m\boldsymbol{r})(t)$$

which reduces to Eq. (1.1.9) in the non-relativistic limit.

III. **"actio = reactio"**: Forces between any two objects in a given system are always equal and opposite.

- The word action in this context refers to the force exerted by one object on another. For extended objects, the forces refer to the forces exerted on the individual centers of mass.[1]

[1] The use of the phrase "action" in this sense is a reflection of the times at which Newton formulated his axioms where many concepts we are using today had not yet been introduced. Today we speak of forces and reserve the word action for the time integral over the Lagrangian of a physical system, see Sec. 2.

- In a system of n objects we may label the objects with an integer index $i \in \{1, \ldots, n\}$ and denote the force that the particle i exerts on particle k by $\boldsymbol{F}_{ik}$. In this case "actio = reactio" states that

$$\boldsymbol{F}_{ik} = -\boldsymbol{F}_{ki} \tag{1.1.11}$$

- A full description of a physical system must, in principle, take into account all forces between all objects in the universe, since generically they all interact with each other: clearly an impossible task.

  Solvable physics problems usually focus in on a small part of our world that can be reasonably dealt with (i) in complete isolation, or (ii) whose back reaction onto the rest of the world or objects of interest is negligible.

  - (i) is justifiable if the forces exerted from *external* objects on the objects in the system we wish to isolate for simplicity's sake (to be called *external forces*) are (very) much smaller than the forces between the particles included in the system (to be called *internal forces*).
  - (ii) would apply if comparable forces within a system we have already isolated from the rest of the universe are involved, but one of the objects still under consideration is extremely heavy, so that

$$\ddot{\boldsymbol{r}}_{\text{heavy}}(t) = \sum_i \boldsymbol{F}_{i\text{heavy}}/M_{\text{heavy}} \approx 0 \ . \tag{1.1.12}$$

    This implies that the dynamics and trajectory of the heavy particle is not affected by the forces exerted by the other particles. The heavy particle can then be conveniently deemed *external* and the back reaction on its motion be ignored.

  A slightly different case of playing with system "boundaries" is encountered in the two-body problem with internal forces. This can be reduced to an effective one-body problem through separation of the center- of-mass motion, where a fictitious particle of mass $\mu = \frac{m_1 m_2}{m_1+m_2}$ moves in the field of an external force, which simplifies the discussion tremendously.

Note that the Eq. (1.1.11) still holds, despite (1.1.12), and that the induced change of momentum of the heavy particle is of the same order as that of the light particles: $\dot{\boldsymbol{p}}_{\text{heavy}}(t) = \sum_i \boldsymbol{F}_{i\text{heavy}}$

1.2 Inertial frames and Galilei transformations

With the existence of inertial frames assured by Newton's first law and the notion of independence of frame built into it, the question arises how many different inertial frames there are and how they might differ.

There are two types of restrictions that constrain the transformations between inertial frames

- The properties of space (homogeneity and isotropy) and time (homogeneity) need to be respected in *all* frames, including inertial ones.

- Among the remaining transformations, transformations from one inertial frame to another must take an inertial trajectory into another, i.e. if in inertial frame A a trajectory $\boldsymbol{x}^A(t)$ satisfies $\ddot{\boldsymbol{x}}^A(t) = 0$, its representation $\boldsymbol{x}^B(t)$ in another inertial frame must satisfy $\ddot{\boldsymbol{x}}^B(t) = 0$.

We will analyze this in turn:

- **Restrictions on frame changes imposed by homogeneity and isotropy:**

- **Time:** We have already seen how to answer this question for time measurements in inertial frames (ignoring relativity!): The time measurements in two inertial frames may differ by

$$t_i^B = \lambda^{BA} t_i^A + \beta^{BA} \qquad \lambda^{BA} = \pm 1 \qquad \beta^{BA} \in \mathbb{R} \tag{1.2.1}$$

which already gives us infinitely many inertial frames B that can be constructed from a single frame B we start with. What we do know, however, is that the time components of *any* pair of inertial frames are connected in this way so that Eq. (1.2.1) gives a full account of all of these.

- **Space:** The spatial transformations admit a similar classification: The transformations of $\mathbb{E}^3$ that preserve its vector space nature are the linear maps from $\mathbb{R}^3$ into itself. These can be represented by 3×3 matrices, elements of $\mathbb{R}^{3\times 3}$. This allows for

$$\boldsymbol{x}^B = R^{BA} \boldsymbol{x}^A \qquad R^{BA} \in \mathbb{R}^{3\times 3} \tag{1.2.2}$$

Notation alert: the lower indices $i = 1, 2$ label objects, not vector components!

If we require that the measurement of length differences and relative angles in two inertial frames A and B be the same, we obtain a further condition on the matrix R^{BA}. The requirement just stated in words is

$$\langle \boldsymbol{x}_1^A - \boldsymbol{x}_2^A, \boldsymbol{y}_1^A - \boldsymbol{y}_2^A \rangle \stackrel{!}{=} \langle \boldsymbol{x}_1^B - \boldsymbol{x}_2^B, \boldsymbol{y}_1^B - \boldsymbol{y}_2^B \rangle \tag{1.2.3}$$

where $\boldsymbol{x}_i^B = R^{BA} \boldsymbol{x}_i^A$ and $\boldsymbol{y}_i^B = R^{BA} \boldsymbol{y}_i^A$.
Since $R^{BA}\boldsymbol{x}_1^A - R^{BA}\boldsymbol{x}_2^A = R^{BA}(\boldsymbol{x}_1^A - \boldsymbol{x}_2^A)$ we can introduce the shorthand $\boldsymbol{x}^{A,B} := \boldsymbol{x}_1^{A,B} - \boldsymbol{x}_2^{A,B}$ (likewise for $\boldsymbol{y}_i$) and check if the condition

$$\langle \boldsymbol{x}^B, \boldsymbol{y}^B \rangle \stackrel{!}{=} \langle \boldsymbol{x}^A, \boldsymbol{y}^A \rangle \qquad \forall \;\; \boldsymbol{x}^A, \boldsymbol{y}^A \in \mathbb{R}^3 \; . \tag{1.2.4}$$

further restricts R^{BA}.
Suppressing the labels on R^{BA} for simplicity we get

$$\langle \boldsymbol{x}^B, \boldsymbol{y}^B \rangle = (\boldsymbol{x}^B)^t \cdot \boldsymbol{y}^B = (R\boldsymbol{x}^A)^t \cdot R\boldsymbol{y}^A = (\boldsymbol{x}^A)^t R^t \cdot R\boldsymbol{y}^A \stackrel{!}{=} (\boldsymbol{x}^A)^t \cdot \boldsymbol{y}^A = \langle \boldsymbol{x}^A, \boldsymbol{y}^A \rangle \tag{1.2.5}$$

where the operational statement is

$$(\boldsymbol{x}^A)^t R^t \cdot R\boldsymbol{y}^A \stackrel{!}{=} (\boldsymbol{x}^A)^t \cdot \boldsymbol{y}^A \qquad \forall \;\; \boldsymbol{x}^A, \boldsymbol{y}^A \in \mathbb{R}^3 \; . \tag{1.2.6}$$

Since this must hold for all $\boldsymbol{x}^A, \boldsymbol{y}^A \in \mathbb{R}^3$ as stated we find that

$$R^t \cdot R \stackrel{!}{=} \mathbb{1} \qquad \text{or} \qquad R^t = R^{-1} \tag{1.2.7}$$

As we will see below, this is precisely the statement that R is a rotation in three dimensions (up to a possible switch from a right handed to a left handed coordinate system), an element of what we will learn to call $\mathsf{O}(3)$, the orthogonal group in three dimensions.
Aside from these quite specific linear transformations, Eq. (1.2.3) is constructed to also allow for translations

$$\boldsymbol{x}_i^B = \boldsymbol{x}_i^A + \boldsymbol{\alpha}^{BA} \qquad \boldsymbol{y}_i^B = \boldsymbol{y}_i^A + \boldsymbol{\alpha}^{BA} \qquad \boldsymbol{\alpha}^{BA} \in \mathbb{R}^3 \; . \tag{1.2.8}$$

Since these directly drop in the differences

$$\boldsymbol{x}_1^B - \boldsymbol{x}_2^B = (\boldsymbol{x}_1^A + \boldsymbol{\alpha}^{BA}) - (\boldsymbol{x}_2^B + \boldsymbol{\alpha}^{BA}) = \boldsymbol{x}_1^A - \boldsymbol{x}_2^A \tag{1.2.9}$$

We still need to understand that these are indeed rotations!

even before we insert these into the scalar products of Eq. (1.2.3).
Combining rotations R and translations $\boldsymbol{\alpha}$ we obtain the most general form of a transformation between two frames in a homogeneous and isotropic space in the form

$$\boldsymbol{x}^B = R \cdot \boldsymbol{x}^A + \boldsymbol{\alpha} \qquad R \in \mathbb{R}^{3\times 3} \;\text{ with }\; R^t \cdot R = \mathbb{1}\;; \quad \boldsymbol{\alpha} \in \mathbb{R}^3[\text{length}] \tag{1.2.10}$$

Why not one but the other?

At this point both R and α must be independent of spatial coordinates, but they may depend on time!
A time dependence in α may indicate that the frames move against each other, possibly show a relative acceleration. A time dependence or R indicates that the frames are rotating against each other in a time dependent manner.

Consider frames attached to two moving cars on a winding road. They will experience both relative acceleration and rotations.

Definition 1 – moving frames, rest frames, comoving frames – nomenclature:
I have been a bit loose with name dropping in the above: We have encountered frames attached to objects: these are conventionally called co-moving frames or rest frames of the object in question.

Transformations between inertial frames must guarantee $\ddot{\boldsymbol{x}}^A(t) = 0 \Leftrightarrow \ddot{\boldsymbol{x}}^B(t) = 0$:

More precisely: if an object moves uniformly (without acceleration) in inertial frame A (its trajectory $\boldsymbol{x}(t)$ in terms of A-coordinates satisfies $\ddot{\boldsymbol{x}}^A(t) = 0$) then it must move uniformly in *any* other inertial coordinate system B i.e. its trajectory $\boldsymbol{x}(t)$ in terms of B-coordinates satisfies $\ddot{\boldsymbol{x}}^B(t) = 0$.

- Clearly this requirement does not affect the time transformations of Eq. (1.2.1).
- For Eq. (1.2.10) this is different, if we consider $\boldsymbol{x}^A(t)$ to be the trajectory of an inertial object:
  At this point we have no reason to exclude the possibility that both R and $\boldsymbol{\alpha}$ may be time dependent.
  Thus, differentiating twice with respect to time, we obtain

$$\ddot{\boldsymbol{x}}^B(t) = \frac{d^2}{dt^2}\left(R \cdot \boldsymbol{x}^A + \boldsymbol{\alpha}\right) = \ddot{R}(t)\boldsymbol{x}^A(t) + 2\dot{R}(t)\dot{\boldsymbol{x}}^A(t) + R(t)\ddot{\boldsymbol{x}}^A(t) + \ddot{\boldsymbol{\alpha}}(t) \stackrel{!}{=} 0 \tag{1.2.11}$$

  $\ddot{\boldsymbol{x}}^A(t) = 0$ holds by assumption, so that

$$\boldsymbol{x}^A(t) = \boldsymbol{r}_0 + \boldsymbol{v}_0 t \tag{1.2.12}$$

  with *arbitrary* vectors $\boldsymbol{r}_0$ and $\boldsymbol{v}_0$: the conditions must hold for any conceivable inertial motion.
  Using Eq. (1.2.12), the condition (1.2.11) reads

$$\ddot{R}(t)(\boldsymbol{r}_0 + \boldsymbol{v}_0 t) + 2\dot{R}(t)\boldsymbol{v}_0 + \ddot{\boldsymbol{\alpha}}(t) \stackrel{!}{=} 0 \qquad \forall \boldsymbol{r}_0, \boldsymbol{v}_0, t$$

  This can only vanish for *all* $\boldsymbol{r}_0$ and $\boldsymbol{v}_0$ if the terms vanish individually for *all* times t. We read off that

$$\ddot{R}(t) = 0 \;\text{ and }\; \dot{R}(t) = 0 \;\Rightarrow\; R \;\text{ is constant in time} \tag{1.2.13}$$

  and

$$\ddot{\boldsymbol{\alpha}}(t) = 0 \;\Rightarrow\; \boldsymbol{\alpha}(t) = \boldsymbol{a} + \boldsymbol{w}t \tag{1.2.14}$$

where $\boldsymbol{a} \in \mathbb{R}^3[\text{length}]$ is an fixed offset between the two frames at $t = 0$ and $\boldsymbol{w} \in \boldsymbol{R}^3[\frac{\text{length}}{\text{time}}]$ is a constant relative velocity between the inertial frames.

The most general spatial transformation between two inertial frames then is

$$\boldsymbol{x}^B = R \cdot \boldsymbol{x}^A + \boldsymbol{a} + \boldsymbol{w}t \qquad R \in \mathsf{O}(3)\ ,\ \boldsymbol{a} \in \mathbb{R}^3[\text{length}]\ , \boldsymbol{w} \in \mathbb{R}^3[\frac{\text{length}}{\text{time}}] \tag{1.2.15}$$

where the *only* time dependence is in the relative motion term $\boldsymbol{w}t$.

The combined set of transformations (1.2.10) and (1.2.15) describe the complete set of transformations between *any* pair of inertial frames.

Summary 1.1 – Inertial frames and Galilei transformations:

We conclude that the the most general transformation that relates two inertial frames A and B that is compatible with Newtons first law is the combined set of transformations

$$t^B = \lambda t^A + \beta \qquad \lambda = \pm 1\ ,\ \beta \in \mathbb{R}[\text{time}] \tag{1.2.16a}$$

$$\boldsymbol{x}^B = R \cdot \boldsymbol{x}^A + \boldsymbol{a} + \boldsymbol{w}t \qquad R \in \mathsf{O}(3)\ ,\ \boldsymbol{a} \in \mathbb{R}^3[\text{length}]\ , \boldsymbol{w} \in \mathbb{R}^3[\frac{\text{length}}{\text{time}}] \tag{1.2.16b}$$

with fixed (time independent) relative orientation R, and constant offset $\boldsymbol{a}$ and fixed relative velocity $\boldsymbol{w}$.

Since *all* inertial frames are mutually related in this manner, we can start from any one of them and view all others as created from it via a Galilei transformation. Thus, Eq. (1.2.16a) provides a full classification of inertial frames, there is a unique one for each unique Galilei transformation.

Aside 1.2 – There is no time dependence in the analogue of R and α in relativity:

In special as well a general relativity, there is only a single invariance condition that contains *both* space and time coordinates *simultaneously*,

$$c^2(t_1^B - t_2^B)^2 - (\boldsymbol{x}_1^B - \boldsymbol{x}_2^B)^2 \stackrel{!}{=} c^2(t_1^A - t_2^A)^2 - (\boldsymbol{x}_1^A - \boldsymbol{x}_2^A)^2 \tag{1.2.17}$$

and the corresponding transformation that respects homogeneity and isotropy is forced to be independent of *both* space and time coordinates, just as the rotations and translations in (1.2.10) had to be independent of the spatial coordinates.

The special rôle of Cartesian coordinates vs curvilinear coordinates:

Cartesian coordinates correspond to ON bases of our $\mathbb{E}^3$, they ideally represent the vector space nature of $\mathbb{R}^3$. We may well choose to parametrize the points in space using curvilinear coordinates, spherical, cylindrical, or any other variant, but the vector space nature is only manifest in Cartesian coordinates. We therefore sharpen our notion of a frame to a Cartesian system.

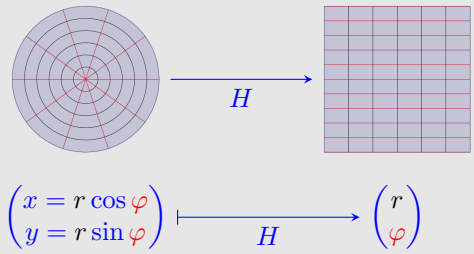
Non-Cartesian coordinate systems will play a rôle in solving differential equations in a given frame, but they are not helpful in discussing the classification of all ways to connect coordinate systems that satisfy invariance conditions tailored to impose homogeneity and isotropy.

Reminder 1.2 – curvilinear coordinate systems on $\mathbb{R}^3$:

.. are generically smooth invertible maps (diffeomorphisms) (for our purpose at least C^2) from an open subset U of $\mathbb{R}^3$ into $\mathbb{R}^3$:

$$H : U \subset \mathbb{R}^3 \to \mathbb{R}^3 \tag{1.2.18}$$

that "put a coordinate net onto U" – polar coordinates may serve as an example:



$$\begin{pmatrix} x = r\cos\varphi \\ y = r\sin\varphi \end{pmatrix} \xmapsto{H} \begin{pmatrix} r \\ \varphi \end{pmatrix}$$

Note how the coordinate net is "straightened" out on the right. This is also the way coordinate systems are introduced for manifolds M in general where $U \subset M$ might have little to do with an $\mathbb{F}^n$, directly, but the image is always in $\mathbb{F}^n$ for either $\mathbb{F} = \mathbb{R}$ or $\mathbb{C}$. In the example given here physicists tend to think about $H^{-1} : (\varphi, r) \mapsto (r\cos\varphi, r\sin\varphi)$, not H as the defining relationship.

1.3 Mathematical interlude: matrix Lie groups

We have now repeatedly relied on the interpretation or R as a rotation. To understand why this is the case and to prepare for later applications we need a little heavier mathematical machinery and a short look at Lie groups. Applications of Lie groups in physics are ubiquitous, Noether's theorem that governs conservation laws is but the first example you will encounter. The discussion of conservation laws in classical and quantum mechanics are all based on symmetry considerations that all rely on the theory of groups. The Standard Model of Particle Physics cannot even be phrased without recourse to its symmetry groups as it defines its particle content.

This will also give us the means to see that the set of Galilei transformations actually forms a Lie group.

1.3.1 Matrix Lie groups with applications in classical and quantum mechanics

Let me first note that the sets of matrices

$$\mathsf{GL}(n, \mathbb{F}) := \{A \in \mathbb{F}^{n\times n} | \det A \neq 0, \text{i.e. } A \text{ invertible}\} \tag{1.3.1}$$

for $\mathbb{F} = \mathbb{C}, \mathbb{R}$ form groups (of matrices -with matrix multiplication as the composition). To avoid the need to specify a basis we might alternatively define this as the group of invertible linear maps $\mathsf{GL}(V)$ from V to V where V is a $\mathbb{F}$-vector space. These are called the General Linear groups of $\mathbb{F}^n$ or V respectively. Both definitions lead to the same construct (isomorphic groups).

Definition 2 – Matrix Lie groups:

A matrix Lie group is any subgroup H of $\mathsf{GL}(n;\mathbb{F})$ with the property that any series of matices A_n in H that converges to a matrix $A \in \mathbb{F}^{n\times n}$ has either $A \in H$ or A is not invertible.

Convergence here utilizes the topological structure on $\mathbb{F}^{n\times n}$. Note that this includes $\mathsf{GL}(n;\mathbb{F})$ itself.

The definition is equivalent to the statement that H be a closed subgroup of $\mathsf{GL}(n;\mathbb{F})$ under the specified topology and exlcudes any form of discreteness in the topology used. This rules out all discrete subgroups with countable numbers of elements but goes beyond that somewhat simplified notion as the following example shows:

Example 1.1 – continuous versus closed – the role of topology:

Take an irrational number a and consider the the group

$$H := \{\begin{pmatrix} e^{it} & \\ & e^{ita} \end{pmatrix} | t \in \mathbb{R}\} \subset \mathsf{T}^2 := \{\begin{pmatrix} e^{it} & \\ & e^{is} \end{pmatrix} | t, s \in \mathbb{R}\} \subset \mathsf{GL}(2;\mathbb{C}) \tag{1.3.2}$$

H is a subgroup of the torus group T^2 and in fact traces out a dense subset on the Torus, a line that never closes on itself.Most importantly, such a line comes arbitrarily close to to any point on the torus, but will not reach all of the points, just like the rational numbers can approximate any real number arbitrarily well without containing them all. For example, H does not contain $-\mathbb{1}_{2\times 2}$, but we can construct a sequence A_n that converges to it in the standard topology of $\mathbb{C}^{2\times 2}$.

The group H can, however, be given a different topology, in which the distance between two points $h_1, h_2 \in H$ is defined as the length of the shortest path "in the group H" joining h_1 to h_2. In this topology, H is identified homeomorphically with the real line by identifying each element with the number θ in the definition of H. With this topology, H is just the group of real numbers under addition and is therefore a Lie group, even a matrix Lie group if we employ the affine trick.

Reminder 1.3 – groups:

A group $(G,\cdot)$ is a pair, consisting of a set G and an composition operation

$$\begin{aligned} \cdot : G \times G &\to G \\ (a,b) &\mapsto a\cdot b\ . \end{aligned} \tag{1.3.3}$$

Furthermore, there must be a neutral element $1_G \in G$ (often denoted simply as 1) such that $1_G \cdot a = a$ for all $a \in G$ and for each $a \in G$ there must exist an inverse a^{-1} such that $a^{-1}a = 1_G$. Lastly the composition must be associative, i.e. $a(bc) = (ab)c$ for all $a, b, c \in G$.

In fact, if 1_G is a left neutral element ($1_G \cdot a = a$), then it is also right neutral ($a \cdot 1_G = a$) and a left inverse ($a^{-1}a = 1_G$) is also automatically a right inverse ($aa^{-1} = 1_G$).

Note that to verify that $(G,\cdot)$ is a group once a set and an operation are given, one must not only look

for neutral elements and inverses, one must also verify that in fact $a \cdot b \in G$ for all $a, b \in G$. This is to make sure that in fact $\cdot : G \times G \to G$.

The notation used here is referred to as the multiplicative notation, alternatively one often encounters an additive notation which replaces $\cdot$ by $+$,1 by 0, and a^{-1} by $-a$. In the multiplicative case the multiplication dot is often omitted when writing "products."

Reminder 1.4 – subgroup:

A subgroup H of a group G is a subset, that is itself a group with the composition inherited from G. This requires the unit element of G to lie in H, as well as $a \in H \Leftrightarrow a^{-1} \in H$ and that H is closed under the group operation: $ab \in H \ \forall \ a, b \in H$. (Associativity is inherited from G.)

Matrix Lie groups have infinitely many elements and they from smooth geometric objects called differentiable manifolds. This insight provides quite powerful tools to prove certain properties and gives rise to a new level of insights, such as the possibility to generalize the concept of to that of Lie groups, which no longer need a reference to matrix spaces. We will, however, avoid the additional layer of complexity for our purposes.

We will be first interested in unitary and orthogonal groups, whose definitions are formally

$$\mathsf{U}(n) := \{A \in \mathsf{GL}(n, \mathbb{C}) | A^\dagger A = 1\} \tag{1.3.4}$$

$$\mathsf{O}(n) := \{A \in \mathsf{GL}(n, \mathbb{R}) | A^t A = 1\} \tag{1.3.5}$$

where the conditions imply that the associated canonical scalar products are preserved under $x \mapsto Ax$.

Check that this is indeed the case.

Reminder 1.5 – canonical scalar products on $\mathbb{R}^n$:

The canonical scalar product in $\mathbb{R}^n$ is given by

$$\begin{aligned} \langle , \rangle : \mathbb{R}^n \times \mathbb{R}^n &\to \mathbb{R} \\ (\boldsymbol{u}, \boldsymbol{v}) &\mapsto \langle \boldsymbol{u}, \boldsymbol{v} \rangle := \boldsymbol{u}^t \cdot \boldsymbol{v} \end{aligned} \tag{1.3.6}$$

This is positive definite ($\langle \boldsymbol{u}, \langle \boldsymbol{u} \rangle > 0$ for all $\boldsymbol{u} \in \mathbb{R}^n \setminus \{\boldsymbol{0}\}$) and bilinear (linear in both the first $[\langle \alpha \boldsymbol{u} + \beta \boldsymbol{v}, \boldsymbol{w} \rangle = \alpha \langle \boldsymbol{u}, \boldsymbol{w} \rangle + \beta \langle \boldsymbol{v}, \boldsymbol{w} \rangle]$ and second components $[\langle \boldsymbol{u}, \alpha \boldsymbol{v} + \beta \boldsymbol{w} \rangle = \alpha \langle \boldsymbol{u}, \boldsymbol{v} \rangle + \beta \langle \boldsymbol{u} \boldsymbol{w} \rangle]$ for all $\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \in \mathbb{R}^n$ and $\alpha, \beta \in \mathbb{R}$).

Reminder 1.6 – canonical scalar products on $\mathbb{C}^n$:

The canonical scalar product in $\mathbb{C}^n$ is given by

$$\begin{aligned} \langle , \rangle : \mathbb{R}^n \times \mathbb{R}^n &\to \mathbb{R} \\ (\boldsymbol{u}, \boldsymbol{v}) &\mapsto \langle \boldsymbol{u}, \boldsymbol{v} \rangle := \boldsymbol{u}^\dagger \cdot \boldsymbol{v} \end{aligned} \tag{1.3.7}$$

This is again positive definite ($\langle \boldsymbol{u}, \boldsymbol{u} \rangle > 0$ for all $\boldsymbol{u} \in \mathbb{C}^n \setminus \{\boldsymbol{0}\}$) and sesquilinear (anti-linear in the first component $[\langle \alpha \boldsymbol{u} + \beta \boldsymbol{v}, \boldsymbol{w} \rangle = \alpha^* \langle \boldsymbol{u}, \boldsymbol{w} \rangle + \beta^* \langle \boldsymbol{v}, \boldsymbol{w} \rangle]$ and linear in the second component $[\langle \boldsymbol{u}, \alpha \boldsymbol{v} + \beta \boldsymbol{w} \rangle =$

$\alpha\langle \boldsymbol{u}, \boldsymbol{v} + \beta\langle \boldsymbol{u}, \boldsymbol{w}\rangle]$ for all $\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \in \mathbb{C}^n$ and $\alpha, \beta \in \mathbb{C}$).

Concepts 1.1 – What's in a name – orthogonal groups:

If we inspect the defining relations of orthogonal and unitary groups in component notation,

$$A^t_{ik} A_{kj} = A_{ki} A_{kj} \stackrel{!}{=} \delta_{ij} \qquad \text{and} \qquad A^\dagger_{ik} A_{kj} = A^*_{ki} A_{kj} \stackrel{!}{=} \delta_{ij} \tag{1.3.8}$$

after choosing an orthonormal basis to specify the components, we need only to recognize that $[\boldsymbol{a}^{(i)}]_k := A_{ki}$ denotes the k-th component of the i-th column vector of the matrix A (recall: these column vectors are the images of the basis vectors under the linear map represented by A) In terms of column vectors (1.3.8) states that

$$(\boldsymbol{a}^{(i)})^t \cdot \boldsymbol{a}^{(j)} \stackrel{!}{=} \delta_{ij} \qquad \text{and} \qquad (\boldsymbol{a}^{(i)})^\dagger \cdot \boldsymbol{a}^{(j)} \stackrel{!}{=} \delta_{ij} \tag{1.3.9}$$

i.e. the column vectors form an orthonormal set with respect to the respective scalar product: A maps the basis vectors onto a new orthonormal set of image vectors.

For both groups, taking the determinant of $A^\dagger A = 1$ and $A^t A = 1$ respectively, we find that

$$|\det(A)|^2 = 1 \ . \tag{1.3.10}$$

This shared property has very different implications in the two cases:

- For $\mathsf{O}(n)$, the determinants are real and there are only two real numbers with modulus one:

  $$\det(A) = \pm 1 \ . \tag{1.3.11}$$

  This implies that, topologically, the $\mathsf{O}(n)$ groups consist of (at least) two disconnected components. The "special" groups $\mathsf{SO}(n)$ pick the component with $\det(A) = 1$, the component that contains the unit element (the other component does not contain the unit element and hence does not form a group by itself).

- For $\mathsf{U}(n)$ group elements and determinants are complex: $(\det(A))^* \det(A) \stackrel{!}{=} 1$ implies that $\det(A)$ lies on the unit circle

  $$\det(A) = e^{i\phi} \qquad \text{with } \phi \in \mathbb{R}. \tag{1.3.12}$$

  This condition does *not* split the group into disconnected components.

  We note instead that $A = e^{i\alpha} \mathbb{1}_n$ is an element of $\mathsf{U}(n)$. This states that we can read $U(1) = \{e^{i\alpha} | \alpha \in \mathbb{R}\}$ as a subgroup of $\mathsf{U}(n)$ (as the image of the embedding homomorphism that takes $e^{i\alpha} \mapsto e^{i\alpha}\mathbb{1}$).

  As in the real case we may still impose the additional condition $\det(A) = +1$ and define another subgroup of $\mathsf{U}(n)$, the special unitary group $\mathsf{SU}(n)$.

  The two subgroups $\mathsf{U}(1)$ and $\mathsf{SU}(n)$ of $\mathsf{U}(n)$ overlap: $\mathsf{SU}(n)$ contains a (discrete and Abelian) subgroup of "pure phases", known as its center $\{e^{2\pi i r/n}\mathbb{1}_{n\times n} | r \in (0 : n-1)\} \cong \mathbb{Z}_n$, the subgroup that commutes with all group elements.

We will see below that at least the Lie algebras behave accordingly.

As a result we see that every element in $\mathsf{U}(n)$ can be written as the product of a phase and a unitary matrix with determinant $+1$: For every $A \in \mathsf{U}(n)$ we know that $(\det A)^{-\frac{1}{n}} A \in \mathsf{SU}(n)$ and $(\det A)^{\pm\frac{1}{n}} \in \mathsf{U}(1)$. However, the map $A \mapsto (\det A)^{-\frac{1}{n}}$ from $\mathsf{U}(n) \to \mathsf{U}(1)$ is not onto, it misses the roots of unity. For this reason $\mathsf{U}(n) = \mathsf{U}(1) \times \mathsf{SU}(n)/\mathbb{Z}_n$.

For the record: the definitions for the special unitary and orthogonal groups are

$$\mathsf{SU}(n) := \{A \in \mathsf{GL}(n,\mathbb{C}) | A^\dagger A = 1, \det(A) = 1\} \tag{1.3.13}$$

$$\mathsf{SO}(n) := \{A \in \mathsf{GL}(n,\mathbb{R}) | A^t A = 1, \det(A) = 1\} \tag{1.3.14}$$

Aside 1.3 – the ϵ-tensor (permutation symbol) as a group invariant; the Leibniz formula:

$\epsilon^{i_1 \dots i_n} = \text{signature}(\{i_1, \dots, i_n\}) = \epsilon(\sigma)$ is the signature of the permutation $\sigma : \{1, \dots, n\} \mapsto \{i_1, \dots, i_n\}$, i.e. it is 1 if the permutation is even, -1 if it is odd and 0 if any of the entries in $\{i_1, \dots, i_n\}$ coincide.

The determinant can be expressed in terms of an alternating sum over permutations with the signs of the individual terms determined by the signature of the permutation (Leibniz formula):

$$\det(A) = \sum_{\sigma \in S_n} \epsilon(\sigma) A_{1\sigma(1)} \cdots A_{n\sigma(n)} = \epsilon_{j_1 \dots j_n} A_{1 j_1} \cdots A_{n j_n} \tag{1.3.15}$$

where S_n is the permutation group of a set of n objects. The second expression on the right uses the definition of the ϵ-tensor (verify term by term!).

Note that reshuffling the indices that are held fixed on the right hand side of Eq. (1.3.15) according to $\{1, \dots, n\} \mapsto \{i_1, \dots, i_n\}$ leads to a simple change of sign according to

$$\epsilon_{j_1 \dots j_n} A_{i_1 j_1} \cdots A_{i_n j_n} = \epsilon_{i_1 \dots i_n} \epsilon_{j_1 \dots j_n} A_{1 j_1} \cdots A_{n i_n} = \epsilon_{i_1 \dots i_n} \det(A) \tag{1.3.16}$$

This version of the Leibniz formula exhibits the ϵ-tensor in n-dimensions as an invariant of all groups with unit determinants, in particular of $\mathsf{SU}(n)$ and $\mathsf{SO}(n)$.

Verify this for $n = 2, 3$.

The Leibniz formula is often used to show that $\det A = \det A^t$ if you have trouble finding a reference in the literature.

Aside 1.4 – defining Lie groups by tensor invariants:

The definitions of $\mathsf{O}(n)$ and $\mathsf{U}(n)$ used above can be rephrased: $\mathsf{O}(n)$ and $\mathsf{U}(n)$ are the (respectively real or complex) matrix groups that leave δ^{ij} (in n-dimensions) invariant:

$$A^t_{ik} \delta_{kl} A_{lj} = A_{ki} A_{kj} \stackrel{!}{=} \delta_{ij} \qquad \text{and} \qquad A^\dagger_{ik} \delta_{kl} A_j = A^*_{ki} A_{kj} \stackrel{!}{=} \delta_{ij} \tag{1.3.17}$$

$\mathsf{SO}(n)$ and $\mathsf{SU}(n)$are the (respectively real or complex) matrix groups groups that leave both δ^{ij} (in n-dimensions) and $\epsilon_{i_1 \dots i_n}$ (i.e. the determinant) invariant:

$$A_{i_1 j_1} \cdots A_{i_n j_n} \epsilon_{j_1 \dots j_n} \stackrel{\text{Leibniz formula for det}}{=} \det(A) \epsilon_{i_1 \dots i_n} \stackrel{\det(A)=1}{=} \epsilon_{i_1 \dots i_n} \tag{1.3.18}$$

This is the stance taken, for example, in Cvitanović's book.

Definition 3 – Lie algebras of matrix Lie groups:
For matrix Lie groups $\mathsf{G} \subset \mathsf{GL}(n, \mathbb{F})$ one may define the Lie-algebra of the group as

$$\mathsf{g} := \{X \in \mathbb{F}^{n\times n} | e^{sX} \in \mathsf{G}\ \forall s \in \mathbb{R}\} \tag{1.3.19}$$

Note that $s \in \mathbb{R}$ even when $\mathbb{F} = \mathbb{C}$ in this definition. To justify the name, we have to show that this set indeed forms a (real) algebra, i.e. that it is a vector space over the real numbers, and in addition there is the notion of a product in this algebra (a map from $\mathsf{g} \times \mathsf{g} \to \mathsf{g}$ that is linear in both factors).

Concepts 1.2 – the exponential map exp : $\mathbb{K}^{n\times n} \to \mathsf{GL}(n, \mathbb{K})$:
The exponential map of matrices

$$\begin{aligned} \exp : \mathbb{K}^{n\times n} &\to \mathsf{GL}(n, \mathbb{K}) \\ X &\mapsto e^X := \sum_{n=0} \frac{X^n}{n!} \end{aligned} \tag{1.3.20}$$

is generally well defined and satisfies

$$(e^X)^{-1} = e^{-X} \tag{1.3.21}$$

since $[X, X] = 0$. This justifies our choice of target space.

Calculating e^X: This relies on the fact that any element X of $\mathbb{K}^{n\times n}$ can be decomposed into a sum of a diagonalizable and a nilpotent term. To see that refer to the Jordan normal form and write $X = SJS^{-1}$ and decompose J into a sum of its diagonal part D and what remains of it (all above the diagonal): $J = D + N$. (In fact it is enough to know that on can find a J that is zero *below* the diagonal.) For N, there is a *finite* $m \in \mathbb{N}$ such that $N^{m+1} = 0$ (proof by induction in the dimension n). On top of that $[D, N] = 0$ for any two matrices of that form. Then we can separately calculate

$$e^{SDS^{-1}} = \sum_{k=1}^{\infty} \frac{1}{k!} \underbrace{(SDS^{-1})(SDS^{-1}) \cdots (SDS^{-1})}_{k \text{ factors of } SDS^{-1}} = Se^D S^{-1} \quad e^D \text{trivially exponentiates} \tag{1.3.22a}$$

$$e^{SNS^{-1}} = Se^N S^{-1} = S \sum_{k=1}^{m} \frac{N^k}{k!} S^{-1} \quad \textit{finite} \text{ number of terms only!} \tag{1.3.22b}$$

The two results combine into

$$e^X = e^{S(D+N)S^{-1}} = Se^{D+N}S^{-1} = Se^D e^N S^{-1} \quad \text{since } [D, N] = 0 \tag{1.3.22c}$$

which provides us with the knowledge that e^X exists for all X (no convergence issues at all) and a means to calculate it. That is what Mathematica uses in its `MatrixExp` function.

A more general definition of Lie groups that steps beyond matrix Lie groups recognizes the groups as differentiable manifolds and interprets the Lie-algebras as the tangent spaces at the unit element. This immediately identifies the latter as real vector spaces whose dimension defines the dimension of the manifold.

By differentiating w.r.t. s one the finds from $A^\dagger A = 1$ or $A^t A = 1$ that

$$\frac{d}{ds}A^\dagger(s)A(s) = 0 \xrightarrow{@s=0} X^\dagger = -X \qquad \text{and} \qquad \frac{d}{ds}A^t(s)A(s) = 0 \xrightarrow{@s=0} X^t = -X \tag{1.3.23}$$

and

$$\det(A(s)) = e^{\mathrm{tr}(sX)} \overset{!}{=} 1 \;\Rightarrow \mathrm{tr}(X) = 0 \qquad \text{(see Eq. (1.3.28))} \tag{1.3.24}$$

which allows us to characterize the Lie-algebras of the unitary and orthogonal groups alternatively as

$$\mathsf{u}(n) := \{X \in \mathbb{C}^{n\times n} | X^\dagger = -X\} \neq \mathsf{su}(n) := \{X \in \mathbb{C}^{n\times n} | X^\dagger = -X,\ \mathrm{tr}(X) = 0\} \tag{1.3.25}$$

where we note that $\mathsf{u}(n)$ is genuinely larger than its subspace $\mathsf{su}(n)$, but

$$\mathsf{o}(n) = \{X \in \mathbb{R}^{n\times n} | X^t = -X\} = \mathsf{so}(n) := \{X \in \mathbb{R}^{n\times n} | X^t = -X,\ \mathrm{tr}(X) = 0\} \tag{1.3.26}$$

since $X^t = -X$ automatically implies $\mathrm{tr}(X) = 0$. Note that these are indeed vector-spaces over the real numbers in all cases, *not* the complex numbers: We see at a glance that linear combinations of such objects with real coefficients retain the stated properties. How about complex linear combinations? Linear combinations with *complex* coefficients break $X^\dagger = -X$ outright in the unitary case. They simply fall out of $\mathbb{R}^{n\times n}$ in the orthogonal case.

Remark 1.1 – Why on earth is $\det(e^X) = e^{\mathrm{tr}(X)}$?:
To prove this, use $X = S(D+N)S^{-1}$ to find

$$\begin{aligned} \det e^X &= \det(S)\det(e^D)\det(e^N)\frac{1}{\det S} = \det(e^D)\det(e^N) \\ &\overset{\text{Eq. (1.3.28)}}{=} e^{\mathrm{tr}(D+N)} = e^{\mathrm{tr}S(D+N)S^{-1}} = e^{\mathrm{tr}X} \end{aligned} \tag{1.3.27}$$

Where the key steps are:

$$\det(e^D) = e^{m_i\lambda_i} = e^{\mathrm{tr}D} \qquad \lambda_i \text{ the eigenvalues, } m_i \text{ their multiplicities} \tag{1.3.28a}$$

$$\det(e^N) = 1 = e^{\mathrm{tr}N} \qquad \text{since } N \text{ and all } N^k \text{ live } \textit{above the diagonal}\text{, i.e. } e^N \text{ is upper diagonal with ones on the diagonal: } \det(e^N) = 1\text{, but also } \mathrm{tr}N = 0 \tag{1.3.28b}$$

As a vector space, it is spanned by a basis, whose members are usually referred to as the generators of the group, since upon exponentiation, they "generate" a group element. At least some of the group elements can be "generated" from the algebra through the exponential map.

Can all group elements be generated in this way? Are there any obvious obstacles?

Beyond the vector space structure (addition as the composition, the null vector as a neutral element, $-\boldsymbol{v}$ as the inverse to $\boldsymbol{v}$ under addition, multiplication by real numbers) there is also a multiplication defined in this space, defined with the help of matrix multiplication, the commutator:

› **Lemma 1 – The commutator provides a (non-Abelian) product for the Lie algebra:**
If X, Y are in some Lie algebra g, then so is also their commutator

$$[X, Y] := XY - YX \in \mathsf{g} \tag{1.3.29}$$

This is the product that turns g into an algebra. Note that there is no mention of a neutral element or inverses! In particular: neither XY nor YX are usually in g.

(1.3.29) is based on an observation that is interesting in its own right, namely that

$$X \in \mathsf{g} \Leftrightarrow AXA^{-1} \in \mathsf{g} \tag{1.3.30}$$

for all $A \in G$, simply because $e^{s\,AXA^{-1}} = A\,e^{sX}A^{-1} \in G$ for all real s. From there, note that $e^{sX}Ye^{-sX}$ describes a smooth curve in the vector space g, whose derivative at any point along the curve lies itself in that vector space. (View the derivative as a limiting process to verify this.) Hence

$$\mathsf{g} \ni \frac{d}{ds}\bigg|_{s=0} e^{sX}Ye^{-sX} = XY - YX = [X, Y]$$

as claimed.

› **Remark 1.2 – physics convention for Lie algebra elements:**
Note that in physics, the convention is to write e^{isM} instead of e^{sX} for *both* the unitary and orthogonal groups. This sets $M = -iX$ which becomes completely imaginary in the orthogonal case where X has real coefficients. The conditions (1.3.23) then turn into $M^\dagger = M$ for both the unitary and orthogonal groups. Both such matrices are diagonalizable and have *real* eigenvalues – therefore, in quantum mechanics, they may correspond to *observables*. (Think angular momentum for $\mathsf{SO}(3)$ or spin for $\mathsf{SU}(2)$.) Without the link to quantum mechanical observables, the appearance of completely imaginary Lie-algebras for the completely real groups $\mathsf{SO}(n)$ is a little contrived – mathematicians tend to avoid it.

1.3.2 Parametrizing the Lie algebras of unitary and orthogonal groups, dimensions

Parameter counting yields the number of independent real degrees of freedom in the Lie-algebra (its dimension as a vector space).

› $\mathsf{u}(n)$ **and** $\mathsf{su}(n)$**:** Anti-Hermitean generators are generically of the form

$$X = -X^\dagger = \begin{pmatrix} ib_{11} & -a_{12} + ib_{12} & \cdots & -a_{1n} + ib_{1n} \\ a_{12} + ib_{12} & ib_{22} & & \\ \vdots & & \ddots & \\ a_{1n} + ib_{1n} & & & ib_{nn} \end{pmatrix} \tag{1.3.31}$$

Since we are interested separately in the case with and without trance, let me split the trace part off:

$$X = -X^\dagger = i\alpha \underbrace{\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix}}_{\substack{= 0 \text{ unless } \mathsf{u}(n) \\ \text{generates } \mathsf{U}(1) \subset \mathsf{U}(n)}} + \underbrace{\begin{pmatrix} ib_{11} & a_{12}+ib_{12} & \cdots & a_{1n}+ib_{1n} \\ -a_{12}+ib_{12} & ib_{22} & & \\ \vdots & & \ddots & \\ -a_{1n}+ib_{1n} & & & -i\sum_{k=1}^{n-1} b_{kk} \end{pmatrix}}_{\text{traceless, fully in } \mathsf{su}(n)} \tag{1.3.32}$$

Formally redefines all new b_{ii} as shifted by $-\alpha$ ...

with real α, a_{ij}, and b_{ij}. We read off that the Lie algebra of $\mathsf{U}(n)$ can be viewed as the sum of those of $\mathsf{U}(1)$ and $\mathsf{SU}(n)$:

$$\mathsf{u}(n) = \mathsf{u}(1) \oplus \mathsf{su}(n) \tag{1.3.33}$$

Counting the independent real parameters we have

- 1 real parameter if there is a non-vanishing trace allowed ($\mathsf{u}(n)$ only)
- $n-1$ on the diagonal of the traceless part
- two times (for a and b) $(n-1)+(n-2)+\ldots+1 = \sum_{k=1}^{n-1} k = \frac{n(n-1)}{2}$ above the diagonal (those below are then already fixed)

i.e. we have

- $\dim(\mathsf{su}(n)) = n-1+2\times\frac{n(n-1)}{2} = n^2-1$, while $\dim(\mathsf{u}(n)) = n^2$.

each dimension given by the number of free parameters allowed.

› $\mathsf{o}(n) = \mathsf{so}(n)$**:** This emerges from the previous case by setting all imaginary parts, i.e. α and all $b_{ij} \to 0$. The result

$$X = -X^t = \begin{pmatrix} 0 & -a_{12} & \cdots & -a_{1n} \\ a_{12} & 0 & & \\ \vdots & & \ddots & \\ a_{1n} & & & 0 \end{pmatrix}, \tag{1.3.34}$$

has only $\frac{n(n-1)}{2}$ independent real parameters.

1.3.3 Orthogonal and unitary Lie-groups and algebras, a summary

	unitary: $x^\dagger y \stackrel{!}{=} (Ax)^\dagger (Ax)$		**orthogonal:** $x^t y \stackrel{!}{=} (Ax)^t (Ax)$	
The groups	$A \in \mathsf{GL}(n,\mathbb{C}),\ A^\dagger A = 1$	defines $A \in \mathsf{U}(n)$	$A \in \mathsf{GL}(n,\mathbb{R}),\ A^t A = 1$	defines $A \in \mathsf{O}(n)$
	$\lvert\det(A)\rvert^2 = \det(A^\dagger)\det(A) = 1$		$\lvert\det(A)\rvert^2 = \det(A^t)\det(A) = 1$	
	$\Rightarrow \det(A) = e^{i\alpha}\ \forall\ A \in \mathsf{U}(n)$		$\Rightarrow \det(A) = \pm 1\ \forall\ A \in \mathsf{O}(n)$	two conn. comp.
	$A \in \mathsf{GL}(n,\mathbb{C}),\ A^\dagger A = 1,\ \det(A) = +1$	defines $A \in \mathsf{SU}(n)$	$A \in \mathsf{GL}(n,\mathbb{R}),\ A^t A = 1,\ \det(A) = +1$	defines $A \in \mathsf{SO}(n)$
The Lie algebras	$\forall\ s \in \mathbb{R},\ A(s) := e^{sX} \stackrel{!}{\in} \mathsf{U}(n)$	$\Rightarrow A \in \mathsf{SU}(n)$	$s \in \mathbb{R},\ A(s) := e^{sX} \stackrel{!}{\in} \mathsf{O}(n)$	$\Rightarrow A \in \mathsf{SO}(n)$
	$\frac{d}{ds} A^\dagger(s)A(s) = 0\ \forall s \in \mathbb{R}$ both $\mathsf{U}(n)$ and $\mathsf{SU}(n)$	$\Rightarrow X^\dagger = -X\ \in \mathbb{C}^{n\times n}$	$\frac{d}{ds} A^\dagger(s)A(s) = 0\ \forall s \in \mathbb{R}$ both $\mathsf{O}(n)$ and $\mathsf{SO}(n)$	$\Rightarrow X^t = -X\ \in \mathbb{R}^{n\times n}$
	$\det(A(s)) = e^{s\ \mathrm{tr}X} = 1$ for $\mathsf{SU}(n)$	$\Rightarrow \mathrm{tr}X = 0$	$\det(A(s)) = e^{s\ \mathrm{tr}X} = 1$ redundant	$\mathrm{tr}X = 0$ automatic
		$\mathsf{u}(n) = \mathsf{u}(1) \oplus \mathsf{su}(n)$		$\mathsf{so}(n) = \mathsf{o}(n)$
	$\dim(\mathsf{u}(n)) = n^2$	$\dim(\mathsf{su}(n)) = n^2 - 1$		$\dim(\mathsf{so}(n) = \frac{n(n-1)}{2}$

From Wikipedia (*much more there*): Marius Sophus Lie (17 December 1842 – 18 February 1899) was a Norwegian mathematician. He largely created the theory of continuous symmetry, and applied it to the study of geometry and differential equations.



Another main contributor to the theory of Lie groups was Elie Cartan:

From Wikipedia (*much more there*): Élie Joseph Cartan (9 April 1869 – 6 May 1951) was an influential French mathematician, who did fundamental work in the theory of Lie groups and their geometric applications. He also made significant contributions to mathematical physics, differential geometry, and group theory. He was the father of another influential mathematician, Henri Cartan.



From Wikipedia (*much more there*): Gottfried Wilhelm Leibniz (sometimes von Leibniz) (July 1, 1646 – November 14, 1716) was a German mathematician and philosopher. He wrote in different languages, primarily in Latin (40%), French (30%) and German (15%). Leibniz occupies a prominent place in the history of mathematics and the history of philosophy. He developed the infinitesimal calculus independently of Isaac Newton, and Leibniz's mathematical notation has been widely used ever since it was published.



1.3.4 Special properties of $\mathsf{SU}(2)$ and $\mathsf{SO}(3)$

Both $\mathsf{SU}(2)$ and $\mathsf{SO}(3)$ are connected and compact, and the exponential map reaches all elements, i.e. all elements in this group can be written in the form $A = e^X$ where X lies in the associated Lie algebra. The two Lie algebras are usually written in terms of specific bases, the Pauli-matrices for $\mathsf{su}(2)$ and the totally antisymmetric tensor for $\mathsf{so}(3)$:

› **Pauli-matrices and $\mathsf{su}(2)$:** $\mathsf{su}(2)$ is $2^2-1=3$-dimensional. The canonical basis for $\mathsf{su}(2)$ ($\{it^a, a=1,2,3\}$ in mathematical convention, drop the i for physics conventions) is usually given in terms of Pauli matrices $\{\sigma^a, a=1,2,3\}$

$$it^a := i\sigma^a/2 \qquad \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1.3.35}$$

Note that the t^a and the Pauli matrices σ^a are Hermitean (such that it^a is anti-Hermitean).

It is easy to verify that

$$[t^a, t^b] = i\epsilon^{abc}t^c \tag{1.3.36}$$

proving that the Lie algebra is indeed closed under commutation. Similarly

$$\{t^a, t^b\} := t^a t^b + t^b t^a = \frac{1}{2}\delta^{ab}\mathbb{1} \tag{1.3.37}$$

and

$$\frac{1}{2}\mathrm{tr}((t^a)^\dagger t^b) = 1 \tag{1.3.38}$$

Since the whole group can be reached by the exponential map, a general element

$$e^{i\omega^a t^a} = \mathbb{1}\cos(\frac{|\boldsymbol{\omega}|}{2}) + 2i\hat{\omega}^a t^a \sin(\frac{|\boldsymbol{\omega}|}{2}) \tag{1.3.39}$$

is fully characterized by the vector $\boldsymbol{\omega} \in \mathbb{R}^3$.

› **The canonical basis of $\mathsf{so}(3)$:** $\mathsf{so}(3)$ is $\frac{3(3-1)}{2} = 3$-dimensional and the canonical basis elements can be written as

$$(it^a)^{kl} = \epsilon^{kal} \qquad \text{i.e.} \qquad it^1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \quad it^2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \quad it^3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{1.3.40}$$

These are basis elements of the Lie algebra.

Since they are elements of the Lie-algebra, their mutual commutators can be expanded as linear combinations of basis elements. This exercise yields

$$[t^a, t^b] = i\epsilon^{abc}t^c \qquad \text{(summation convention for } c\text{!)} \tag{1.3.41}$$

A general element of $\mathsf{SO}(3)$ characterized by the vector $\boldsymbol{\varphi} = (\varphi_1, \varphi_2, \varphi_2)^t$ [$\hat{\boldsymbol{\varphi}}$ prescribes the rotation axis, $|\boldsymbol{\varphi}|$ the rotation angle], can be written as

$$R^{ij}(\boldsymbol{\varphi}) = \left(e^{\varphi^a i t^a}\right)^{ij} = \hat{\varphi}^i\hat{\varphi}^j + (\delta^{ij} - \hat{\varphi}^i\hat{\varphi}^j)\ \cos(|\boldsymbol{\varphi}|) + \hat{\varphi}^k\epsilon^{ikj}\ \sin(|\boldsymbol{\varphi}|) \tag{1.3.42}$$

where R^{ij} are the components of the rotation matrix. If we let R act on a specific vector we may alternatively write

$$R(\boldsymbol{\varphi})\cdot\boldsymbol{x} = (\hat{\boldsymbol{\varphi}}\cdot\boldsymbol{x})\ \hat{\boldsymbol{\varphi}} - \cos(\varphi)\ \hat{\boldsymbol{\varphi}}\times(\hat{\boldsymbol{\varphi}}\times\boldsymbol{x}) - \sin(\varphi)\ \hat{\boldsymbol{\varphi}}\times\boldsymbol{x} \tag{1.3.43}$$

The three terms are easy to interpret:

- The first term
  - projects onto the direction of the rotation axis (it selects the component in the direction of $\boldsymbol{\varphi}$ and then
  - leaves that component unchanged.

  A rotation does not affect the component of a vector pointing in the direction of the rotation axis.
- The $(\delta_{ij} - \hat{\varphi}_i\hat{\varphi}_j)$ second term is a projection operator onto the plane perpendicular to $\boldsymbol{\varphi}$ in which the rotation takes place. In this place it acts like a unit matrix (eigenvalues 1). This carries the cosine factor.
- The third term also only affects components of vectors living in the plane perpendicular to $\boldsymbol{\varphi}$ (since $\hat{\varphi}_k\epsilon_{ikj}\hat{\varphi}_j = 0$). This term corresponds to the off diagonal contributions that must carry the sine factor.

For illustration, consider the case $\hat{\boldsymbol{\varphi}} = (1,0,0)^t$ and note that the corresponding matrix in this case is

$$\begin{aligned} R((1,0,0)^t) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \cos(|\boldsymbol{\varphi}|) + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \sin(|\boldsymbol{\varphi}|) \\ &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(|\boldsymbol{\varphi}|) & -\sin(|\boldsymbol{\varphi}|) \\ 0 & \sin(|\boldsymbol{\varphi}|) & \cos(|\boldsymbol{\varphi}|) \end{pmatrix} \end{aligned} \tag{1.3.44}$$

Warning 1.1 – Not all elements of any Lie group can be written in the form e^X part I:
An obvious obstacle exists for $\mathsf{O}(n)$ for any element with $\det A = -1$, since $\det e^X = e^{\mathrm{tr}X} = 1$ for all $X \in \mathsf{o}(n)$. This is simply a consequence of the fact that the component $\det A = -1$ is topologically disconnected from the subgroup $\mathsf{SO}(n)$.

Warning 1.2 – Not all elements of any Lie group can be written in the form e^X part II:
A more sophisticated counter example arises for $\mathsf{SL}(2,\mathbb{R}) := \{A \in \mathbb{R}^{2\times 2} | \det A = 1\}$. Here $\mathsf{sl}(2,\mathbb{R}) := \{X \in \mathbb{R}^{2\times 2} | \mathrm{tr}(X) = 0\}$. The Cayley-Hamilton-Theorem for 2×2-matrices states that $X^2 - \mathrm{tr}(X)X + \det(A)\mathbb{1} = 0$, so that in our case

$$X^2 = -\rho\mathbb{1} \qquad \text{with} \qquad \rho := \det(X) \tag{1.3.45}$$

Exponentiating yields

$$e^X = \begin{cases} \cos(\sqrt{\rho})\mathbb{1} + \frac{\sin(\sqrt{\rho})}{\sqrt{\rho}}X & \rho > 0 \\ \cosh(\sqrt{\rho})\mathbb{1} + \frac{\sinh(\sqrt{\rho})}{\sqrt{\rho}}X & \rho < 0 \\ \mathbb{1} + X & \rho = 0 \end{cases} \tag{1.3.46}$$

From this we find that $\mathrm{tr}e^X \geq -2$ for any $X \in \mathsf{sl}(2,\mathbb{R})$.

Contrast this with

$$\mathsf{SL}(2,\mathbb{R}) \ni A(a) := \begin{pmatrix} -a & 0 \\ 0 & -\frac{1}{a} \end{pmatrix} \qquad \text{(This is a group element, since } \det A = 1 \text{ for all real } a.\text{)} \tag{1.3.47}$$

and note that

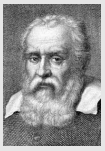
$$\mathrm{tr}(A(a)) = -(a + \frac{1}{a}) < -2 \qquad \text{for all } a > 2 \tag{1.3.48}$$

so that in this case $A(a) \neq e^X$ for any X in $\mathsf{sl}(2,\mathbb{R})$.

It turns out that $\mathsf{SL}(2,\mathbb{R})$ is connected but not compact. The latter turns out to be the reason for the existence of such "non-exponentiated" elements although a derivation of that result requires more abstract arguments.

1.4 The Galilei group – the complete set of transformations that relates any two inertial frames in non-relativistic mechanics

From Wikipedia (*much more there*): Galileo Galilei (15 February 1564 – 8 January 1642), commonly known as Galileo, was an Italian physicist, mathematician, astronomer and philosopher who played a major role in the Scientific Revolution. His achievements include improvements to the telescope and consequent astronomical observations, and support for Copernicanism.



Such a system has a set of symmetries often called the Galilei transformations $G(n)$ (in n-spatial dimensions), given by the *simultaneous* transformation of all coordinates $\boldsymbol{r}_i$ and time t according to

$$G(n) \ni g(R, \boldsymbol{a}, \boldsymbol{w}, s, \lambda) : \begin{pmatrix} t \\ \boldsymbol{r}_i \end{pmatrix} \mapsto \begin{pmatrix} t' = \lambda t + \beta \\ \boldsymbol{r}'_i = R\boldsymbol{r}_i + \boldsymbol{a} + t\boldsymbol{w} \end{pmatrix} \tag{1.4.1}$$

This is constructed using

		# of continuous real parameters	
$\beta \in \mathbb{R}$	temporal translations (energy conservation)	1	(1.4.2a)
$R \in \mathsf{O}(n)$	spatial rotations (angular momentum conservation)	$\frac{n(n-1)}{2} \xrightarrow{n\mapsto 3} = 3$	(1.4.2b)
$\boldsymbol{a} \in \mathbb{R}^n$	spatial translations (conservation of total momentum)	$n \xrightarrow{n\mapsto 3} = 3$	(1.4.2c)
$\boldsymbol{w} \in \mathbb{R}^n$	constant relative motion of two inertial systems (conservation of $\boldsymbol{r}_{\mathrm{cm}}(0) = \boldsymbol{r}_{\mathrm{cm}}(t) - \frac{\sum \boldsymbol{p}_i}{\sum m_i} t$; center of mass principle.) implies that velocities simply add according to $\boldsymbol{v}' = \boldsymbol{v} + \boldsymbol{w}$ as we change inertial systems	$\xrightarrow{n\mapsto 3} = 3$	(1.4.2d)
		$\sum \ldots = 10$ = # of integrals of motion (conservation laws)	

In addition there are two discrete parameters dialed by $|\det R| = \pm 1$ (rotations with or without a reflection at the origin (called parity), and $\lambda = \pm 1$ (-1 corresponds to time reversal). Removing these discrete ones by restricting to $R \in \mathsf{SO}(n=3)$ ($\det R = +1$) and $\lambda = +1$, one arrives at what is called the proper orthochronous Galilei group $G^{\uparrow}_{+}(n=3)$[2].

The underlying invariants are based on the *Euclidean scalar product of* $\mathbb{R}^n$, if only applied to the inter-particle distances (to incorporate the translations, one speaks of the affine subspace of the configuration space)

$$(\boldsymbol{r}_i - \boldsymbol{r}_j)^t \cdot (\boldsymbol{r}_i - \boldsymbol{r}_j) \tag{1.4.3}$$

together with the *independent* invariance of time distances

$$(t_i - t_j)^2 \tag{1.4.4}$$

If we start from these invariants and attempt to *construct* the largest group that respects these two independent constraints, one ends up transformations of the form

$$\begin{pmatrix} t \\ \boldsymbol{r}_i \end{pmatrix} \mapsto \begin{pmatrix} t' = \lambda t + \beta \\ \boldsymbol{r}'_i = R\boldsymbol{r}_i + \boldsymbol{a} \end{pmatrix} \tag{1.4.5}$$

Remark 1.3:

Note that the "addition of velocities symmetry" is dynamical in nature. It is allowed by the invariants, since Eq. (1.4.3) by itself allows both rotations and translations to be time dependent. (This is excluded in special relativity). The dynamical requirement that $\ddot{\boldsymbol{r}} = 0$ remains true as we transform from one inertial frame to another the condition only restricts to constant rotations but allows time dependent

[2] $\uparrow$ stands for the choice $\lambda = +1$, the $+$ stands for $\det R = +1$.

space translations of the form $\boldsymbol{\alpha} = \boldsymbol{a} + \boldsymbol{w}t$.

One may simply do that by checking composition laws, looking for the neutral element and inverses.

Assume that $\alpha(t) = \frac{1}{2}\boldsymbol{a}t^2$. What is the relative acceleration of the frames? What is the fictitious force in frame B. (Assume that the particle is moving inertially in frame A.)

1.5 Arbitrary frames including non-inertial frames, fictitious forces

Arbitrary frames including non-inertial frames are related by

$$t^B = \lambda t^A + \beta \qquad \lambda = \pm 1\ ,\ \beta \in \mathbb{R}[\text{time}] \tag{1.5.1a}$$

$$\boldsymbol{x}^B = R(t)\cdot \boldsymbol{x}^A + \boldsymbol{\alpha}(t) \qquad R(t) \in \mathsf{O}(3)\ ,\ \boldsymbol{\alpha}(t) \in \mathbb{R}^3[\text{length}] \text{ for all } t \tag{1.5.1b}$$

- *Any* time dependence in $R(t)$ leads to a non-inertial frame. For example an $R(t)$ that corresponds to a rotation with constant angular velocity leads to a frame B that rotates with that constant velocity and a fictitious force, a Coriolis force induced by the time derivatives of R.
- If $\alpha(t)$ is not of the form $\boldsymbol{a} + \boldsymbol{w}t$ the transformation describes a situation in which the two frames are accelerated with respect to each other.

Coriolis and centrifugal forces are apparent forces that appear in a rotating frame, a special case of Eq. (1.5.1a) in which the non-inertial frame rotates around a fixed axis $\hat{\boldsymbol{\omega}}$ with fixed angular velocity:

$$t^B = t^A =: t \tag{1.5.2a}$$

$$\boldsymbol{x}^B = R(t)\cdot \boldsymbol{x}^A \qquad R(t) = e^{(\omega^a i t^a)t} \in \mathsf{SO}(3) \tag{1.5.2b}$$

Please take care to distinguish the time variable t from the basis elements of $\mathsf{so}(3)$ labeled t^a.

To explore the consequences of Eq. (1.5.2) we consider the trajectory $\boldsymbol{x}(t)$ of a test particle of mass m in both frames and compare the EsOM expressed in terms of $\boldsymbol{x}^A(t)$ and $\boldsymbol{x}^B(t)$.

We consider B to be the inertial frame and A to be the rotating frame. Then we know that in frame B, there is no acceleration unless a force $\boldsymbol{F}^B$ acts on the particle:

$$m\ddot{\boldsymbol{x}}^B(t) = \boldsymbol{F}^B(t) \tag{1.5.3}$$

The equations of motion in the two frames must be related by

$$m\ddot{\boldsymbol{x}}^B(t) = m\frac{d^2}{dt^2}R(t)\cdot\boldsymbol{x}^A(t) = m\ddot{R}(t)\boldsymbol{x}^A(t) + m2\dot{R}(t)\dot{\boldsymbol{x}}^A(t) + mR(t)\ddot{\boldsymbol{x}}^A(t) \tag{1.5.4}$$

By virtue of Eq. (1.5.3), the l.h.s. equals the force in the original inertial frame B, the last term contains the acceleration in the rotating frame $\ddot{\boldsymbol{x}}^A(t)$ we wish to determine. Solving for $m\ddot{\boldsymbol{x}}^A(t)$ we obtain

$$m\ddot{\boldsymbol{x}}^A(t) = R^{-1}(t)\left[\underbrace{m\ddot{\boldsymbol{x}}^B(t)}_{\boldsymbol{F}^B(t)} - m\ddot{R}(t)\boldsymbol{x}^A(t) - m2\dot{R}(t)\dot{\boldsymbol{x}}^A(t)\right] \tag{1.5.5}$$

We see that in frame A, the particle is still accelerated by the original force already present in frame B via the term

$$R^{-1}(t)m\ddot{\boldsymbol{x}}^B(t) = R^{-1}(t)\boldsymbol{F}^B(t) = (F^B(t))^A \tag{1.5.6}$$

The direction of the force is of course affected by the rotation, hence the factor $R^{-1}(t)$. The notation $(F^B(t))^A$ attempts to capture that: the coordinates of the force in system B need to be recast into coordinates in system A.

The two additional terms are have no analogue in an inertial frame, they are artifacts of R being time dependent. They represent apparent forces acting on the particle observed in the rotating frame. To evaluate the $\dot{R}$ and $\ddot{R}$ factors in Eq. (1.5.4) we observe that

$$R^{-1}(t)\cdot\dot{R}(t) = R^{-1}(t)\cdot R(t)\cdot(\omega^a it^a) = \omega^a it^a \tag{1.5.7a}$$

and

$$R^{-1}(t)\cdot\ddot{R}(t) = R^{-1}(t)\cdot R(t)\cdot(\omega^a it^a)^2 = (\omega^a it^a)^2 \tag{1.5.7b}$$

Verify this for yourself!

This follows from the power series representation of $R(\boldsymbol{\omega}t) = e^{(\omega^a it^a)t}$ and the fact that the matrix $\omega^a it^a$ commutes with itself. This allows us to write Eq. (1.5.5) as

$$m\ddot{\boldsymbol{x}}^A = (\boldsymbol{F}^B(t))^A - m(\omega^a it^a)^2\boldsymbol{x}^A(t) - 2m(\omega^a it^a)\dot{\boldsymbol{x}}^A(t) \tag{1.5.8}$$

Note that Scheck is a little sloppy in this definition of the force F^A in the rotating frame in terms of F^B, the force in the inertial frame: the factor R^{-1} is missing!

In this expression, the forces induced by choosing a non-inertial frame are given by

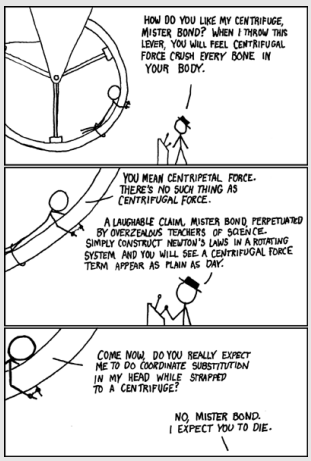
$$\boldsymbol{C} := -2m(\omega^a it^a)\cdot\dot{\boldsymbol{x}}^A(t) = -2m\,\boldsymbol{\omega}\times\boldsymbol{v}^A\ , \qquad \text{the Coriolis force} \tag{1.5.9}$$

and

Generalize this to the case of accelerated rotation, where $R(t) = e^{(\dot{\omega}^a it^a)\omega(t)}$.

$$\boldsymbol{Z} := -m(\omega^a it^a)^2\cdot\boldsymbol{x}^A(t) = -m\,\boldsymbol{\omega}\times(\boldsymbol{\omega}\times\boldsymbol{x}^A)\ , \qquad \text{the centrifugal force.} \tag{1.5.10}$$

Remark 1.4 – semantic wars about the existence of fictitious forces:



Centripetal forces are a perfectly good description for what is going on in the situation depicted on the right, provided we use an *inertial* frame to do so. In the accelerated frame, motion of objects will in general look different and often more complicated: particles and objects that are not subject to acceleration in an inertial frame will appear to undergo acceleration (velocity changes) from the perspective of the accelerated observer. These are accounted for by what is unfortunately called fictitious forces that appear in the equation of motion in the non-inertial frame.

Imagine an experiment set up in a closed windowless cabin on a centrifuge (or an elevator for that matter) that enables you to measure forces acting on your apparatus. This will reveal the (net) forces acting, but offer not information about the nature of the forces observed.

If we do not know a priory, if a frame is inertial or not, all forces we can measure in an experiment may well contain fictitious contributions.

From the perspective of general relativity objects objects falling down an evacuated tube in earth's gravitational field are in free fall: they experience no force. This is precisely what parajumpers experience – a feeling of weightlessness (up to frictional forces against air resistance).

A person standing on the surface of the earth is experiencing a force excerted by the surface they are standing on.

1.6 Simple mechanical systems – definitions of crucial concepts

1.6.1 Closed and open systems and the center of mass principle

A closed n-particle system is a system of n-particles in which the *only* forces acting on the particles are forces between the particles.

We denote the the mass of particle i my m_i and the force that particle i exerts on particle j by $\boldsymbol{F}_{i\to j}$, or more compactly by $\boldsymbol{F}_{ij}$. Any *external* forces on the i-th particle will be denoted by $\boldsymbol{K}_i$. Then we have n equations of motion

$$m_i\ddot{\boldsymbol{r}}_i = \sum_{j\neq i}^{n} \boldsymbol{F}_{ji} + \boldsymbol{K}_i \quad i \in \{1,\dots,n\} \tag{1.6.1}$$

and the assertion that

$$\boldsymbol{F}_{ij} = -\boldsymbol{F}_{ji} \tag{1.6.2}$$

from the action reaction principle.

In the two particle case Eq. (1.6.1) simplifies to the pair of equations

$$m_1\ddot{\boldsymbol{r}}_1 = \boldsymbol{F}_{21} + \boldsymbol{K}_1 \quad \text{and} \quad m_2\ddot{\boldsymbol{r}}_2 = -\boldsymbol{F}_{21} + \boldsymbol{K}_2 \tag{1.6.3}$$

Summing all the equations in (1.6.3), we immediately find that

$$m_1\ddot{\boldsymbol{r}}_1 + m_2\ddot{\boldsymbol{r}}_2 = \boldsymbol{F}_{21} - \boldsymbol{F}_{21} + \boldsymbol{K}_1 + \boldsymbol{K}_2 = \boldsymbol{K}_1 + \boldsymbol{K}_2 \tag{1.6.4}$$

i.e. the internal forces cancel in the sum and the left hand side corresponds to the time derivative of the total momentum of the two particle system, since $\boldsymbol{p}_{\text{total}} = m_1\dot{\boldsymbol{r}}_1 + m_2\dot{\boldsymbol{r}}_2$.

This, in fact generalizes to the n-body system:

$$\begin{aligned}\sum_{i=1}^{n} m_i\ddot{\boldsymbol{r}}_i = \sum_{i=1}^{n}\sum_{j\neq i}^{n}\boldsymbol{F}_{ji} + \sum_i \boldsymbol{K}_i = \quad & \begin{array}{ccccc} 0 & +\boldsymbol{F}_{21} & +\boldsymbol{F}_{31} & +\ldots & +\boldsymbol{F}_{n1} \\ +\boldsymbol{F}_{12} & +0 & +\boldsymbol{F}_{32} & +\ldots & +\boldsymbol{F}_{n2} \\ +\boldsymbol{F}_{13} & +\boldsymbol{F}_{23} & +0 & +\ldots & +\boldsymbol{F}_{n2} \\ \vdots & & & & \\ +\boldsymbol{F}_{1n} & +\boldsymbol{F}_{2n} & & \ldots & +0 \end{array} \\ & + \sum_i \boldsymbol{K}_i \\ = \sum_i \boldsymbol{K}_i & \end{aligned} \tag{1.6.5}$$

due to pairwise cancellation of the internal forces.

The mass weighted combination $\sum_{i=1}^{n} m_i\boldsymbol{r}_i$ is therefore only accelerated if the total external force $\sum_i \boldsymbol{K}_i$ is non-vanishing.

We scale away the mass dimension by dividing out the total mass of the system $m_{\text{total}} := \sum_{i=1}^{n} m_i$ and define the center of mass coordinate

$$\boldsymbol{r}_{\text{cm}} := \frac{\sum_{i=1}^{n} m_i\boldsymbol{r}_i}{\sum_{i=1}^{n} m_i} = \frac{\sum_{i=1}^{n} m_i\boldsymbol{r}_i}{m_{\text{total}}} \tag{1.6.6}$$

Eq. (1.6.5) informs us that $\ddot{\boldsymbol{r}}_{\text{cm}}$ is only nonzero if there are external forces on the system.

This tells us that the total momentum

The last expresses the total momentum in terms of a fictitious particle located at the center of mass!

$$\boldsymbol{p}_{\text{total}} := \sum_{i=1}^{n} \boldsymbol{p}_i = \sum_{i=1}^{n} m_i\dot{\boldsymbol{r}}_i = m_{\text{total}}\dot{\boldsymbol{r}}_{\text{cm}} \tag{1.6.7}$$

is conserved, if the total external force $\sum_i \boldsymbol{K}_i$ zero:

$$\dot{\boldsymbol{p}}_{\text{total}} = \sum_i \boldsymbol{K}_i \quad . \tag{1.6.8}$$

Since the integral operation is linear, the same statement can be made for a mass distributed according to a density function $\rho(\boldsymbol{r})[\frac{\text{mass}}{\text{length}^3}]$ where now

$$\boldsymbol{r}_{\text{cm}} := \frac{1}{m_{\text{total}}} \int_{\mathbb{R}^3} d^3r \; \boldsymbol{r} \; \rho(\boldsymbol{r}) \tag{1.6.9}$$

$$m_{\text{total}} := \int_{\mathbb{R}^3} d^3r \; \rho(\boldsymbol{r}) \tag{1.6.10}$$

This is known as the

› **Center of mass principle:** The center of mass of an n-particle system or a mass distribution behaves like a single particle of mass m_{total} under the influence of a force given by the sum of all external forces.

$$\boldsymbol{p}_{\text{total}} = m_{\text{total}} \dot{\boldsymbol{r}}_{\text{cm}} \qquad \text{where} \qquad \dot{\boldsymbol{p}}_{\text{total}} = \sum_i \boldsymbol{K}_i \tag{1.6.11}$$

For a closed system there are no external forces and the center of mass motion is given by

$$\boldsymbol{r}_{\text{cm}} = \boldsymbol{a} + \boldsymbol{w}t \tag{1.6.12}$$

with constant $\boldsymbol{a} \in \mathbb{R}^3[\text{length}]$ and $\boldsymbol{w} = \boldsymbol{p}_{\text{total}}/m \in \mathbb{R}^3[\frac{\text{length}}{\text{time}}]$

› **Remark 1.5 – Closed two particle systems are special:**
For two particle systems the center of mass becomes $\boldsymbol{r}_{\text{cm}} = \frac{m_1\boldsymbol{r}_1 + m_2\boldsymbol{r}_2}{m_1+m_2}$. To describe all relevant trajectories one may complement this by the relative coordinate $\boldsymbol{r} := \boldsymbol{r}_1 - \boldsymbol{r}_2$, since then

$$\boldsymbol{r}_1 = \boldsymbol{r}_{\text{cm}} + \frac{m_2}{m_1+m_2}\boldsymbol{r} \; ; \qquad \text{and} \qquad \boldsymbol{r}_2 = \boldsymbol{r}_{\text{cm}} - \frac{m_1}{m_1+m_2}\boldsymbol{r} \; ; \tag{1.6.13}$$

Inserting this into the EOM's, we find

$$\mu \ddot{\boldsymbol{r}} = \boldsymbol{F}_{21} \qquad \text{where} \qquad \mu := \frac{m_1 m_2}{m_1+m_2} \tag{1.6.14}$$

is called the reduced mass. By separating the center of mass we have reduced the two-body problem to the motion of one particle with mass μ.

1.6.2 Work and energy

The work done on a particle by a force $\boldsymbol{F}(t)$ in moving a particle along a path $\boldsymbol{r}(t)$ from an initial point $\boldsymbol{r}(t_1)$ to a final point $\boldsymbol{r}(t_2)$ can be defined as the line integral

$$W_{\boldsymbol{r},t_1,t_2} = \int_{\boldsymbol{r},t_1,t_2} d\boldsymbol{r} \cdot \boldsymbol{F} := \int_{t_1}^{t_2} dt \; \boldsymbol{F}(t) \cdot \dot{\boldsymbol{r}}(t) \tag{1.6.15}$$

Newtons second law allows us to connect this to the difference of kinetic energies of the particle at the endpoints by replacing $\boldsymbol{F} \mapsto \dot{\boldsymbol{p}}$ and $\dot{\boldsymbol{r}} \mapsto \boldsymbol{p}/m$:

$$W_{\boldsymbol{r},t_1,t_2} = \int_{t_1}^{t_2} dt\ \dot{\boldsymbol{p}} \cdot \boldsymbol{p}/m = \frac{1}{2m} \int_{t_1}^{t_2} dt \frac{d}{dt} \boldsymbol{p}^2 = \frac{1}{2m}(\boldsymbol{p}^2(t_2) - \boldsymbol{p}^2(t_1)) = T(t_2) - T(t_1) \tag{1.6.16}$$

A priori, the integral in Eq. (1.6.15) would appear to depend both on the endpoints and the detailed shape of the trajectory connecting the two points.

If the work does not depend on the path but only on the endpoints, the force is called conservative. There are three equivalent ways to characterize a conservative force field (defined everywhere in space or in a simply connected volume in space)

$$\boldsymbol{\nabla} \times \boldsymbol{F} = \boldsymbol{0} \qquad \text{the curl of the force is zero} \tag{1.6.17a}$$

$$W_{\boldsymbol{r}_{\text{closed}}} = \oint dt\ \boldsymbol{F}(t) \cdot \dot{\boldsymbol{r}}(t) = 0 \qquad \text{no net work is done if a particle is moved along a closed path} \tag{1.6.17b}$$

$$\boldsymbol{F}(\boldsymbol{r}) = -\boldsymbol{\nabla} U(\boldsymbol{r}) \qquad \text{the force can be written as the gradient of a potential} \tag{1.6.17c}$$

In this case we find that work is also related to the difference of potential energy, by noting that

$$\frac{d}{dt} U(\boldsymbol{r}(t)) = \boldsymbol{\nabla} U \cdot \dot{\boldsymbol{r}} \tag{1.6.18}$$

so that if $\boldsymbol{F}(\boldsymbol{r}) = -\boldsymbol{\nabla} U(\boldsymbol{r})$ we have an alternative expression for the work done that reads

$$W_{\boldsymbol{r},t_1,t_2} = \int_{t_1}^{t_2} dt \boldsymbol{F} \cdot \dot{\boldsymbol{r}} = -\int_{t_1}^{t_2} dt \boldsymbol{\nabla} U \cdot \dot{\boldsymbol{r}} = -\int_{t_1}^{t_2} dt \frac{d}{dt} U(\boldsymbol{r}(t)) = -\big(U(\boldsymbol{r}(t_2)) - U(\boldsymbol{r}(t_2))\big) \tag{1.6.19}$$

Derive that $\boldsymbol{F}(\boldsymbol{r}) = -\boldsymbol{\nabla} U(\boldsymbol{r})$ by taking the time derivative in (1.6.20)

$$U(\boldsymbol{r}(t_2)) - U(\boldsymbol{r}(t_1)) = -\int_{\boldsymbol{r},t_1,t_2} d\boldsymbol{r} \cdot \boldsymbol{F} = -(T(t_2) - T(t_1)) \tag{1.6.20}$$

For a single particle system subject to a conservative force this equation is tantamount to *energy conservation*:

$$T(t_2) + U(\boldsymbol{r}(t_2)) = T(t_1) + U(\boldsymbol{r}(t_1)) \tag{1.6.21}$$

Let us consider the slightly more general situation of a many particle system in which the internal forces are conservative, but arbitrary external forces $\boldsymbol{K}_i$ are allowed to act on the i-th particle. The conservative inter-particle forces $\boldsymbol{F}_{ik}$ can only depend on the relative position of the two particles $\boldsymbol{r}_{ik} := \boldsymbol{r}_i - \boldsymbol{r}_k$. They then give rise to potentials

$$U_{ik}(\boldsymbol{r}_{ik}) := -\int_{\boldsymbol{r}_0}^{\boldsymbol{r}_{ik}} d\boldsymbol{r} \cdot F_{ik}(\boldsymbol{r}) \tag{1.6.22}$$

where we have introduced a common reference point $\boldsymbol{r}_0$. This is allowed since we can not measure absolute normalizations of a potential, only potential differences have physics consequences.

Note that

$$U_{ki}(\boldsymbol{r}_{ki}) = -\int_{\boldsymbol{r}_0}^{\boldsymbol{r}_{ki}} d\boldsymbol{r}\cdot F_{ki}(\boldsymbol{r}) = -\int_{\boldsymbol{r}_0}^{-\boldsymbol{r}_{ik}} d\boldsymbol{r}\cdot(-F_{ik}(\boldsymbol{r})) = -\int_{\boldsymbol{r}_0}^{\boldsymbol{r}_{ik}} d\boldsymbol{r}\cdot F_{ik}(\boldsymbol{r}) = U_{ik}(\boldsymbol{r}_{ik}) \tag{1.6.23}$$

such that both $\boldsymbol{F}_{ik}$ and $\boldsymbol{F}_{ki}$ can be written as a derivative of $U_{ik}(\boldsymbol{r}_{ik})$ according to

$$\boldsymbol{F}_{ik} = -\boldsymbol{\nabla}_k U_{ik}(\boldsymbol{r}_{ik}) \qquad \text{and} \qquad \boldsymbol{F}_{ki} = -\boldsymbol{\nabla}_i U_{ik}(\boldsymbol{r}_{ik})) \tag{1.6.24}$$

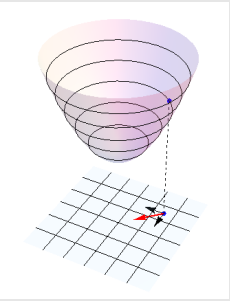
The EOM for the i-th particle in such a system is given by

$$\dot{\boldsymbol{p}}_i = -\boldsymbol{\nabla}_{\boldsymbol{r}_i}\sum_{\substack{k=1\\k\neq i}}^{n} U_{ki}(\boldsymbol{r}_{ki}) + \boldsymbol{K}_i \tag{1.6.25}$$

Remark 1.6 – forces, coordinates, and potentials:

- Single particle case: If we a calculating the force $\boldsymbol{F}(\boldsymbol{r})$ on a particle induced by a potential, we are asking for the change of potential encountered by this particle if we move it against the potential:

$$\boldsymbol{F}(\boldsymbol{r}) = -\boldsymbol{\nabla}_{\boldsymbol{r}} U(\boldsymbol{r})$$



- One particle in the presence of many others: We want to calculate the (sum of the) forces F_{ki} on the particle i we look at the contributions due to the presence of the other particles $k \neq i$.

  Still, the force is due to the change of potential energy of the i-th particle as we move it infinitesimally. We need to take the gradient with respect to its coordinate $\boldsymbol{r}_i$:

$$\boldsymbol{F}_{ki}(\boldsymbol{r}_{ki}) = -\boldsymbol{\nabla}_{\boldsymbol{r}_i} U(\boldsymbol{r}_{ki})$$

We multiply this by $\boldsymbol{p}_i/m_i$ to arrive at an expression that parallels the integrand in Eq. (1.6.16)

$$\dot{\boldsymbol{p}}_i\cdot\boldsymbol{p}_i/m = \frac{d}{dt}\Big(\underbrace{\frac{1}{2m_i}\boldsymbol{p}_i^2}_{=T_i}\Big) = -\frac{1}{m_i}\boldsymbol{p}_i\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_i}\sum_{\substack{k=1\\k\neq i}}^{n} U_{ki}(\boldsymbol{r}_{ki}) + \frac{1}{m_i}\boldsymbol{p}_i\cdot\boldsymbol{K}_i \tag{1.6.26}$$

and we already recognize time derivative of the kinetic energy of the i-th particle. Clearly a sum over all particles will turn that into the time derivative of the total kinetic energy of the system.

The same sum applied to the gradients of the potential energies needs a little thought on how to disentangle

the double sum:

$$\sum_{i=1}^{n}\sum_{\substack{k=1\\k\neq i}}^{n}\dot{\boldsymbol{r}}_i\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_i}U_{ki}(\boldsymbol{r}_{ki})$$

$$\begin{array}{rccccc} = & 0 & +\dot{\boldsymbol{r}}_1\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_1}U_{21}(\boldsymbol{r}_{21}) & +\dot{\boldsymbol{r}}_1\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_1}U_{31}(\boldsymbol{r}_{31}) & +\ldots & +\dot{\boldsymbol{r}}_1\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_1}U_{n1}(\boldsymbol{r}_{n1}) \\ & +\dot{\boldsymbol{r}}_2\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_2}U_{12}(\boldsymbol{r}_{12}) & +0 & +\dot{\boldsymbol{r}}_2\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_2}U_{32}(\boldsymbol{r}_{32}) & +\ldots & +\dot{\boldsymbol{r}}_2\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_2}U_{n2}(\boldsymbol{r}_{n2}) \\ & +\dot{\boldsymbol{r}}_3\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_3}U_{13}(\boldsymbol{r}_{13}) & +\dot{\boldsymbol{r}}_3\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_3}U_{23}(\boldsymbol{r}_{23}) & +0 & +\ldots & +\dot{\boldsymbol{r}}_3\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_3}U_{n3}(\boldsymbol{r}_{n3}) \\ & \vdots & & & & \\ & +\dot{\boldsymbol{r}}_n\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_n}U_{1n}(\boldsymbol{r}_{1n}) & +\dot{\boldsymbol{r}}_n\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_n}U_{n2}(\boldsymbol{r}_{2n}) & & \ldots & +0 \end{array}$$

in which we may pair ij entries with ji entries to find

$$=\sum_{i=1}^{n}\sum_{k=i+1}^{n}\Big(\dot{\boldsymbol{r}}_i\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_i}U_{ki}(\boldsymbol{r}_{ki})+\dot{\boldsymbol{r}}_k\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_k}U_{ik}(\boldsymbol{r}_{ik})\Big)$$

While $\boldsymbol{F}_{ki}=-\boldsymbol{F}_{ik}$, the two terms are projected onto different velocities and do not cancel. Using (1.6.24) we can then write

$$=\sum_{i=1}^{n}\sum_{k=i+1}^{n}\Big(\dot{\boldsymbol{r}}_i\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_i}-\dot{\boldsymbol{r}}_k\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_k}\Big)U_{ki}(\boldsymbol{r}_{ki})$$

and realize that the derivatives in brackets represent a chain rule expression for a time derivative

$$=\sum_{i=1}^{n}\sum_{k=i+1}^{n}\frac{d}{dt}U_{ki}(\boldsymbol{r}_{ki})=\frac{d}{dt}\underbrace{\sum_{i=1}^{n}\sum_{k=i+1}^{n}U_{ki}(\boldsymbol{r}_{ki})}_{=:U\text{ , total potential energy}} \tag{1.6.27}$$

Pulling everything together, we have shown that energy is conserved unless an external force is applied to the system:

› **Energy conservation:** The time derivative of the total energy of the system is equal to the total *power* (work per unit time) of external forces, i.e.

$$\frac{d}{dt}(T+U)(t)=\sum_{i=1}^{n}\dot{\boldsymbol{r}}_i(t)\cdot\boldsymbol{K}_i(t) \tag{1.6.28}$$

where

$$T=\frac{1}{2}\sum_{i=1}^{n}m_i\dot{\boldsymbol{r}}_i^2\ ;\qquad\text{and}\qquad U=\sum_{i=1}^{n}\sum_{k=i+1}^{n}U_{ik} \tag{1.6.29}$$

1.6.3 Central potentials and angular momentum conservation

Central inter-particle potentials, which are a function of only the length of $\boldsymbol{r}_{ik}$

$$U_{ik}(\boldsymbol{r}_{ik})=U_{ik}(|\boldsymbol{r}_{ik}|) \tag{1.6.30}$$

lead to radial forces

$$\boldsymbol{F}_{ik}(\boldsymbol{r}_{ik}) = -\boldsymbol{\nabla}_k U_{ik}(|\boldsymbol{r}_{ik}|) = \underbrace{-\Big(\frac{d}{d|\boldsymbol{r}_{ik}|}U_{ik}(|\boldsymbol{r}_{ik}|)\Big)}_{=:F_{ik}(|\boldsymbol{r}_{ik}|)} \underbrace{\boldsymbol{\nabla}_k|\boldsymbol{r}_{ik}|}_{=\hat{\boldsymbol{r}}_{ik}} \tag{1.6.31}$$

where $F_{ik}(|\boldsymbol{r}_{ik}|)$ a real valued *(Galilei-) scalar* function (invariant under spatial rotations and translations as well as time translations)

By acting with $\boldsymbol{r}_i \times \ldots$ onto the EOM of the i-th particle, we find that

$$m_i \boldsymbol{r}_i \times \ddot{\boldsymbol{r}}_i = \sum_{k\neq i} F_{ki} \boldsymbol{r}_i \times \hat{\boldsymbol{r}}_{ki} + \boldsymbol{r}_i \times \boldsymbol{K}_i \tag{1.6.32}$$

On the left hand side we recognize

$$m\boldsymbol{r}_i \times \ddot{\boldsymbol{r}}_i = \frac{d}{dt} m_i \boldsymbol{r}_i \times \dot{\boldsymbol{r}}_i = \frac{d}{dt}\boldsymbol{r}_i \times \boldsymbol{p}_i = \frac{d}{dt}\boldsymbol{l}_i \tag{1.6.33}$$

Now we sum both sides of the equation over all particles i.e. the index i. The left hand side yields the time derivative of the total angular momentum

$$\boldsymbol{l}_{\text{total}} = \sum_i \boldsymbol{l}_i \tag{1.6.34}$$

The last term, $\sum_i \boldsymbol{r}_i \times \boldsymbol{K}_i$, represents the total external torque on the system

Again the sums in the first right hand term need a closer look

$$\sum_i \sum_{k\neq i} F_{ki} \boldsymbol{r}_i \times \hat{\boldsymbol{r}}_{ki} = \sum_i \sum_{k\neq i} \frac{F_{ki}(|\boldsymbol{r}_{ki}|)}{|\boldsymbol{r}_{ki}|} \boldsymbol{r}_i \times (\boldsymbol{r}_k - \boldsymbol{r}_i) = \sum_i \sum_{k\neq i} \frac{F_{ki}(|\boldsymbol{r}_{ki}|)}{|\boldsymbol{r}_{ki}|} \boldsymbol{r}_i \times \boldsymbol{r}_k = 0 \tag{1.6.35}$$

The cancellations follow the pattern in Eq. (1.6.5) noting that $F_{ki}(|\boldsymbol{r}_{ki}|) = F_{ik}(|\boldsymbol{r}_{ik}|)$ while $\boldsymbol{r}_i \times \boldsymbol{r}_k = -\boldsymbol{r}_k \times \boldsymbol{r}_i$.

This leads to the

› **Principle of angular momentum conservation:** If all inter-particle potentials are rotation symmetric, the total angular momentum remains conserved unless changed by an external torque:

$$\frac{d}{dt}\boldsymbol{l}_{\text{total}} = \sum_i \boldsymbol{r}_i \times \boldsymbol{K}_i \tag{1.6.36}$$

1.6.4 Closed systems and their conservation laws

For closed systems external forces (and thus also external torques) vanish. If the inter-particle potentials are central potentials, i.e. if there is rotational symmetry in the system then the continuous parameters of the

Galilei group match up with the conservation laws of the n-particle systems discussed above:

		# of continuous real parameters	
$\beta \in \mathbb{R}$	temporal translations (conservation of total energy)	1	(1.6.37a)
$R \in \mathsf{O}(n)$	spatial rotations (conservation of total angular momentum)	$\frac{n(n-1)}{2} \xrightarrow{n\mapsto 3} = 3$	(1.6.37b)
$\boldsymbol{a} \in \mathbb{R}^n$	spatial translations (conservation of total momentum)	$n \xrightarrow{n\mapsto 3} = 3$	(1.6.37c)
$\boldsymbol{w} \in \mathbb{R}^n$	constant relative motion of two inertial systems (conservation of $\boldsymbol{r}_{\mathrm{cm}}(0) = \boldsymbol{r}_{\mathrm{cm}}(t) - \frac{\sum \boldsymbol{p}_i}{\sum m_i} t$; center of mass principle.) implies that velocities simply add according to $\boldsymbol{v}' = \boldsymbol{v} + \boldsymbol{w}$ as we change inertial systems	$\xrightarrow{n\mapsto 3} = 3$	(1.6.37d)
		$\sum \ldots = 10$ = # of integrals of motion (conservation laws)	

Is this an accident? That would appear unlikely. We will see that there is a general theorem (by Emmy Noether) that guarantees a conservation law associated with any "contiuous" symmetry of the system. A more precise statement will be postponed to Sec. 5.

1.7 Degrees of freedom, configuration space, and phase space

The number of *degrees of freedom* f in a system of n point particles – the number of coordinates needed to describe the location of all particles at a given time is simply $f = 3n$ (the dimension of space times the number of particles). The space of all particle coordinates

$$\boldsymbol{x}(t) := \begin{pmatrix} \boldsymbol{r}_1(t) \\ \vdots \\ \boldsymbol{r}_n(t) \end{pmatrix} \in \mathbb{R}^{3n}[\text{length}] =: \mathsf{C} \tag{1.7.1}$$

is called the configuration space C

The system as a whole is described by a trajectory in configuration space $\mathsf{C} = \mathbb{R}^{3n}[\text{length}]$, i.e. to fully specify the *state* of a system, it would therefore appear be necessary to prescribe a $3n$-dimensional trajectory as a function of time for *all times*

The trajectories themselves, however, are subject to a coupled set of second order differential equations, whose solutions are fully specified after $2 \cdot 3n$ *initial conditions* (initial locations and velocities) have been selected. If this is true, we only need to specify $2 \cdot 3n = 6n$ real numbers, coordinates and velocities/momenta (in preselected units), of our n particles at a *single* given time in order to fully identify a trajectory. This is an enormous simplification over the need to give $3n$ coordinates for all times: the space of states becomes *finite dimensional* instead of infinite dimensional.

The mathematical formulation used to both phrase the problem and to "enumerate" its solutions uses *phase space* –a space spanned by both coordinates and momenta– instead of configuration space. To make this

more explicit one maps the set of coupled second order differential equations into an equivalent set of first order differential equations, by formally writing them as

$$\dot{\boldsymbol{r}}_i = \boldsymbol{p}_i/m_i \tag{1.7.2a}$$
$$\dot{\boldsymbol{p}}_i = \boldsymbol{F}_i(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_n, \dot{\boldsymbol{r}}_1, \ldots, \dot{\boldsymbol{r}}_n) \tag{1.7.2b}$$

These can be read as a vector equation in $\mathbb{R}^{3n}[\text{length}] \oplus \mathbb{R}^{3n}[\text{momentum}]$, often loosely referred to as a $\mathbb{R}^{6n}$, the space of coordinates and momenta, or *phase space* P by setting

$$\boldsymbol{x} := \begin{pmatrix} \boldsymbol{r}_1 \\ \vdots \\ \boldsymbol{r}_n \\ \boldsymbol{p}_1 \\ \vdots \\ \boldsymbol{p}_n \end{pmatrix} \in \mathbb{R}^{3n}[\text{length}] \oplus \mathbb{R}^{3n}[\text{momentum}] =: \mathsf{P} \qquad \text{and} \qquad \boldsymbol{F} := \begin{pmatrix} \boldsymbol{p}_1/m_1 \\ \vdots \\ \boldsymbol{p}_n/m_n \\ \boldsymbol{F}_1 \\ \vdots \\ \boldsymbol{F}_n \end{pmatrix} \tag{1.7.3}$$

Note that the units on the top $3n$ entries are different from the bottom half. While slightly awkward, this will not interfere with the mathematical statements we are about to make.

so that the whole set of EOMs now reads (in the most general case)

$$\dot{\boldsymbol{x}} = \boldsymbol{F}(\boldsymbol{x}, t) \tag{1.7.4}$$

Remark 1.7 – A point in phase space fully specifies the state of a system:
Eq. (1.7.4) is a first order differential equation, whose solution is fully specified (for all times) by prescribing the value of $\boldsymbol{x}$ (a point in phase space) at some time t_0 (which need not be the initial time).

This leads to another useful way of capturing and thinking about the full sets of solutions to equations of motion of an n-particle system by plotting these solution in phase space (or sections thereof if $n > 1$). The concept is best illustrated by discussing examples for $n = 1$.

1.8 Configuration and phase space at work – examples

1.8.1 Example: The harmonic oscillator

Hooke's law with a spring constant k reads $F(q) = -kq$ and leads to $\omega = \sqrt{k/m}$, our choice of parameters avoids restricting to a spring specifically. Harmonic oscillators appear virtually everywhere in physics!

The harmonic oscillator in one dimension ($n = 1$) is defined by its force law $F(q) = -m\omega^2 q$. Here m has units of mass, ω units of inverse time and q units of length so that the combination indeed has the units of a force. The applied force is proportional to the distance to a reference point (here chosen to be the origin) and is directed so that it always drives the particle back to the reference point. The force is conservative – it arises from a potential energy

$$U(q) = \frac{1}{2} m\omega^2 q^2 \ , \tag{1.8.1}$$

whose existence guarantees energy conservation, a fact we will use below to get insight into the space of solutions with minimal calculational effort.

Newton's second law provides us with a second order differential equation,

$$m\ddot{q} = -m\omega^2 q \tag{1.8.2}$$

which we could solve the "conventional way", by appealing to the mathematical fact that the space of solutions is two dimensional and of the form $q(t) = A_1 e^{\alpha_1 t} + A_2 e^{\alpha_2 t}$, with $\alpha_{1,2}$ determined by inserting this into Eq. (1.8.2) and $A_{1,2}$ still available to accommodate all possible initial conditions. This is demonstrated in remark 1.9. Here I will use the first order formulation, the phase space equations of motion (1.7.4) instead. This way we can in fact *derive* the result directly and see how the two dimensions of the solution space come about.

We write the components of the phase space equations of motion (c.f. (1.7.4)) $\dot{\boldsymbol{x}} = \boldsymbol{F}(\boldsymbol{x})$ using

$$\boldsymbol{x} := \begin{pmatrix} q \\ p \end{pmatrix} \quad \text{and} \quad \boldsymbol{F}(\boldsymbol{x}) = \begin{pmatrix} \frac{p}{m} \\ -m\omega^2 q \end{pmatrix} = \begin{pmatrix} \frac{x_2}{m} \\ -m\omega^2 x_1 \end{pmatrix} \quad \text{so that} \quad \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix} = \begin{pmatrix} \frac{x_2}{m} \\ -m\omega^2 x_1 \end{pmatrix} \tag{1.8.3}$$

or, in matrix form

$$\frac{d}{dt}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 & \frac{1}{m} \\ -m\omega^2 & 0 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \tag{1.8.4}$$

The total energy is conserved and has the form

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 = \frac{x_2^2}{2m} + \frac{1}{2}m\omega^2 x_1^2 \tag{1.8.5}$$

We note that the harmonic oscillator problem has two dimensionful parameters m and ω that can be used to rescale the components of $\boldsymbol{x}$ into objects that have the same dimension (which the current variables do not have!), i.e. by rescaling the components of $\boldsymbol{x}$ into *natural units* of the problem in order to exhibit the prototypical behavior of the system. To this end we define

$$z_1 := \omega\sqrt{m}x_1 \; ; \quad z_2 = \frac{1}{\sqrt{m}}x_2 \; ; \quad \tau := \omega t \tag{1.8.6}$$

Both components of the new variables share the same units, $\boldsymbol{z} \in \mathbb{R}^2[\text{energy}^{\frac{1}{2}}]$ and $\tau \in \mathbb{R}$ is dimensionless.

In the rescaled variables the energy of the system becomes a simple quadratic form

$$E = \frac{\boldsymbol{z}^2}{2} \tag{1.8.7}$$

and the equations of motion become

$$\frac{d}{d\tau}\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = -\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \; . \tag{1.8.8}$$

This equation, to those who understand the exponential map of matrices, has the obvious solution

$$\boldsymbol{z}(\tau) = e^{-(\tau-\tau_0)J}\boldsymbol{z}(\tau_0) = \begin{pmatrix} \cos(\tau-\tau_0) & \sin(\tau-\tau_0) \\ -\sin(\tau-\tau_0) & \cos(\tau-\tau_0) \end{pmatrix}\boldsymbol{z}(\tau_0) \tag{1.8.9}$$

where $\boldsymbol{z}(\tau_0)$ represents the initial condition of the system and

$$J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{1.8.10}$$

is the generator of real rotations in 2d[3]. Initial conditions provided at τ_0 are turned into solutions at τ through a simple clockwise rotation in phase space, accomplished by the matrix

$$e^{-(\tau-\tau_0)J} = \begin{pmatrix} \cos(\tau-\tau_0) & \sin(\tau-\tau_0) \\ -\sin(\tau-\tau_0) & \cos(\tau-\tau_0) \end{pmatrix} \tag{1.8.11}$$

We note that these solutions are the unique solutions that reduce to $\boldsymbol{z}(\tau_0)$ in the limit $\tau \to \tau_0$. A constant additive term would invalidate this feature and break energy conservation. They, in fact represent solutions in moving coordinate systems.

fix this and explain

See the second tutorial

In this formulation energy conservation has turned into a very geometrical feature of the phase space solutions: The length squared of the phase space vector, $\boldsymbol{z}^2$, remains constant for all τ. The trajectories in phase space, the *orbits* of the system, are fully classified by the one conservation law in the system. For higher dimensional systems, where the degrees of freedom outnumber the available conservation laws this will no longer be the case.

Observe that in this example the orbits are fully determined by the *flow map* (or simply flow) of the system

$$\Phi_{\tau,\tau_0} := e^{-(\tau-\tau_0)J} = \begin{pmatrix} \cos(\tau-\tau_0) & \sin(\tau-\tau_0) \\ -\sin(\tau-\tau_0) & \cos(\tau-\tau_0) \end{pmatrix} \tag{1.8.12}$$

and never cross in phase space, see Fig. 1. They correspond to circles of fixed radius (two times the energy

Fix Graphics

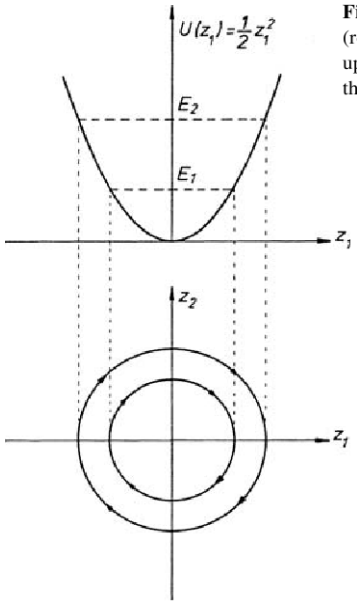


Fig. (redu upper the p

Fig. 1: *Potential and phase portrait for the harmonic oscillator*

of the system), the orbits of the 2-d rotation group. There is one special point: the origin, which represents an *equilibrium point* or *fixed point* a point at which the force (the r.h.s. of the EOM) vanishes.

[3]Read: two-d, meaning two dimensions.

The theory of differential equations proves that this set of observations is not coincidental, it applies (locally in phase space) to all flows.

It is of course easy to reinstate the original variables, the solution then reads

$$\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} \cos(\omega(t-t_0)) & \frac{\sin(\omega(t-t_0))}{m\omega}) \\ -m\omega\sin(\omega(t-t_0)) & \cos(\omega(t-t_0)) \end{pmatrix} \begin{pmatrix} q(t_0) \\ p(t_0) \end{pmatrix} \tag{1.8.13}$$

Comparing to the "conventional" formulation is equally easy, we read off that the trajectory in configuration space is nothing but

$$z_1(\tau) = z_1(\tau_0)\cos(\tau-\tau_0) + z_2(\tau_0)\sin(\tau-\tau_0) \tag{1.8.14}$$

or in the original units

$$q(t) = q(t_0)\cos(\omega(t-t_0)) + \frac{p(t_0)}{m\omega}\sin(\omega(t-t_0)) \tag{1.8.15}$$

Once the full time dependence of the trajectory is known, the momenta simply follow from differentiation as $p(t) = m\dot{q}(t)$ and are usually not mentioned. Note once more how the phase space solution naturally expresses the result in terms of initial conditions, the initial coordinate $q(t_0)$ and the initial momentum $p(t_0)$.

› **Remark 1.8 – Units and plots:**

Note that the result as stated in Eq. (1.8.13) is not universal: it depends on the constants of the situation, it speaks of a mass m and an oscillation frequency ω, and if one were to write this in terms of a spring constant $k = m\omega^2$, even of a specific experiment. To plot the result as in Fig. 1, you have to either:

- do the rescaling of Eq. (1.8.6) in "secret" and put the units including the rescaling factors on the plot axis or, rather desperately
- make several plots for several values of any pair out of m, ω, and k.

1.8.2 Example: The damped harmonic oscillator – an open system

The second order equation for the harmonic oscillator $m\ddot{q} = -m\omega^2 q$ is not the most general second order equation with constant coefficients one can write down. What is missing for that is a force term proportional to the velocity $\dot{q}$, and we introduce such a term by writing

$$m\ddot{q} = -2m\gamma\dot{q} - m\omega^2 q \tag{1.8.16}$$

We have chosen to encode the added freedom using a parameter γ with units of inverse time and have scaled out a factor of m to simplify further manipulations.

If γ in Eq. (1.8.16) is nonzero, the physics of the system is quite different from that encountered before. The system is no longer conservative, the force (sum of terms on the r.h.s.) cannot be derived from a potential. This negates energy conservation: damping dissipates energy away from the harmonic oscillator. A force proportional to velocity $\dot{q}$ is in fact typical for friction, and we are led to interpret the term accordingly. Eq. (1.8.16) describes a damped harmonic oscillator for which a friction term proportional to γ dissipates away energy.

In phase space notation Eq. (1.8.16) reads

$$\frac{d}{dt}\begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} 0 & \frac{1}{m} \\ -m\omega^2 & -2\gamma \end{pmatrix}\begin{pmatrix} q \\ p \end{pmatrix} \ . \tag{1.8.17}$$

Phase space solution: The full solution in phase space emerges by simply integrating

$$\frac{d}{dt}\begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} 0 & \frac{1}{m} \\ -m\omega^2 & -2\gamma \end{pmatrix}\begin{pmatrix} q \\ p \end{pmatrix} \ . \tag{1.8.18}$$

using matrix exponentials. This leads to

$$\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = e^{-\gamma(t-t_0)}\left[\begin{pmatrix} \cos(\sqrt{\omega^2-\gamma^2}(t-t_0)) & \frac{\sin(\sqrt{\omega^2-\gamma^2}(t-t_0))}{m\sqrt{\omega^2-\gamma^2}} \\ -\frac{m\omega^2\sin(\sqrt{\omega^2-\gamma^2}(t-t_0))}{\sqrt{\omega^2-\gamma^2}} & \cos(\sqrt{\omega^2-\gamma^2}(t-t_0)) \end{pmatrix} + \frac{\gamma\sin(\sqrt{\omega^2-\gamma^2}(t-t_0)}{\sqrt{\omega^2-\gamma^2}}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right]\begin{pmatrix} q(t_0) \\ p(t_0) \end{pmatrix} \tag{1.8.19}$$

and can be calculated using the decomposition into $S(D+N)S^{-1}$ outlined in Sec. 1.3 (I have used Mathematica which uses this method to do its work).

To plot the solution one is, once more, better off in rescaled coordinates. Following Eq. (1.8.6) and introducing $s = \gamma/\omega$, the solution reads

$$\begin{pmatrix} z_1(t) \\ z_2(t) \end{pmatrix} = e^{-s(t-t_0)}\left[\begin{pmatrix} \cos(\sqrt{1-s^2}(t-t_0)) & \frac{\sin(\sqrt{1-s^2}(t-t_0))}{\sqrt{1-s^2}} \\ -\frac{\sin(\sqrt{1-s^2}(t-t_0))}{\sqrt{1-s^2}} & \cos(\sqrt{1-s^2}(t-t_0)) \end{pmatrix} + \frac{s\sin(\sqrt{1-s^2}(t-t_0))}{\sqrt{1-s^2}}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right]\begin{pmatrix} z_1(t_0) \\ z_2(t_0) \end{pmatrix} \tag{1.8.20}$$

The presence of the square roots

$$\sqrt{1-s^2} = \sqrt{1-\gamma/\omega} \tag{1.8.21}$$

forces us to consider three qualitatively different cases:

1. $s < 1$ or $\gamma < \omega$ includes the frictionless limit in which $\gamma = 0$ (or $s = 0$). This is known as the underdamped case: there is an overall damping factor $e^{-s(t-t0)}$ that describes the overall energy loss, but oscillatory behavior remains visible; the longer the larger the initial momentum $p(t_0)$ (i.e. the initial kinetic energy carried by the initial condition).
2. $s = 1$ or $\gamma = \omega$ is special. There the cos terms become constant and the sin terms simplify drastically:

$$\cos(\sqrt{1-s^2}(t-t_0)) \xrightarrow{s\to 1} 1 \qquad \text{and} \qquad \frac{\sin(\sqrt{1-s^2}(t-t_0))}{\sqrt{1-s^2}} \xrightarrow{s\to 1} t-t_0 \ . \tag{1.8.22}$$

   No oscillations remain, no matter what the initial conditions are. This is called critical damping.

3. $s > 1$ or $\gamma > \omega$ is even more damped: there $1 - s^2$ becomes negative so that the square root $\sqrt{(1-s^2)} = i\sqrt{s^2-1}$ becomes purely imaginary so that $\sin(ix) = i\sinh(x)$ and $\cos(ix) = \cosh(x)$ replace the oscillating behavior with additional exponentials.

   This is called the overdamped harmonic oscillator.

Note that in all three cases the solutions in terms of the physical initial conditions $\boldsymbol{z}(t_0) \in \mathbb{R}^2[\text{energy}^{\frac{1}{2}}]$ remain real and carry dimension $[\text{energy}^{\frac{1}{2}}]$ for all times. The phase space trajectories for the three cases are are illustrated in Fig. 2.

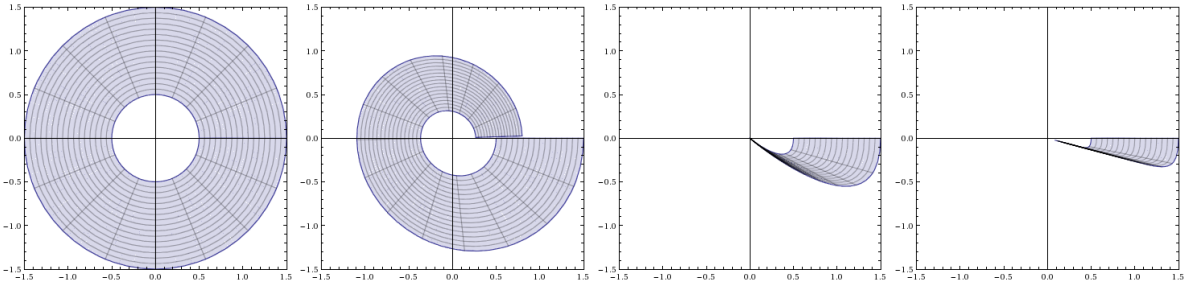


Fig. 2: *From left to right: phase space trajectories of free ($\gamma = 0$), under damped (specifically $\gamma = .1\omega$), critically damped $\gamma = \omega$ and over damped (specifically for $\gamma = 2\omega$) harmonic oscillators. The axis are $z_1 := \omega\sqrt{m}q$, $z_2 = \frac{1}{\sqrt{m}}p$ and the time intervals indicated are equidistant in $\tau := \omega t$.*

› **Remark 1.9 – Solving the harmonic oscillator the "conventional" way:**

A standard textbook would have approached this along a slightly different route: it would have appealed in one way or another, to the theory of differential equations, stating that a linear differential equation of the form

$$\ddot{q} + 2\gamma\dot{q} + aq = 0 \tag{1.8.23}$$

has a two dimensional *complex vector space* of exponential solutions, all of the form

$$q(t) = A_1 e^{\alpha_1 t} + A_2 e^{\alpha_2 t} \tag{1.8.24}$$

provided the α_i are non-degenerate i.e. $\alpha_1 \neq \alpha_2$. If $\alpha_1 = \alpha_2 =: \alpha$ the space of solutions is still two dimensional but the two solutions given in Eq. (1.8.24) are no longer linearly independent, we need a different basis for the space of solutions. In this case the general solution reads

$$q(t) = A_1 e^{\alpha t} + A_2 t e^{\alpha t} \tag{1.8.25}$$

[$e^{\alpha t}$ and $te^{\alpha t}$ are in fact the independent solutions of Eq. (1.8.23) for the case $a = \gamma^2$ which is the place where the degeneracy occurs.]

The ingredients of these solutions are then determined by two very different criteria:

› The α_i are determined by inserting an exponential ansatz $q(t) \mapsto e^{\alpha t}$ into Eq. (1.8.23) to obtain

$$\alpha^2 + 2\gamma\alpha + a = 0 \tag{1.8.26}$$

This is the characteristic equation corresponding to the differential equation (1.8.23), often called the *dispersion relation* of the problem by physicists. The two solutions are readily extracted:

$$\alpha_{1,2} := -\gamma \pm \sqrt{\gamma^2 - a} \tag{1.8.27}$$

and given solely in terms of the constants appearing the characteristic equation. This leads us to two independent basis elements of the space of solutions

$$e_1 := e^{\alpha_1 t} = e^{(-\gamma+\sqrt{\gamma^2-a})t} \qquad \text{and} \qquad e_2 := e^{\alpha_2 t} = e^{(-\gamma-\sqrt{\gamma^2-a})t} \tag{1.8.28}$$

› The superposition coefficients A_i are of a different nature, they serve to select a "point" in solution space and are given by initial conditions. This will be demonstrated below.

Where does our phase-space solution fit? The transformation to phase space is in fact the mathematician's way to show that second order differential equations have a two dimensional space of solutions by reducing them to a coupled set of two first order solutions. The two solutions (1.8.28) arise from the two components of $(q, p)^t$ in the phase space solution.

The special case of $\gamma = 0$, the harmonic oscillator: To compare with Eq. (1.8.24) note that $\gamma = 0$ and $a = \omega^2$. Thus, the general solution reads

$$q(t) = A_1 e^{\sqrt{-\omega^2}t} + A_2 e^{-\sqrt{-\omega^2}t} = A_1 e^{i\omega t} + A_2 e^{-i\omega t} = (A_1 + A_2)\cos(\omega t) - i(A_1 - A_2)\sin(\omega t) \tag{1.8.29}$$

If one is looking for physical solution, one must require that $B_1 := A_1 + A_2$ and $B_2 := -i(A_1 - A_2)$ be *real*, and given by $q(0)$ and $\dot{q}(0)/\omega$ respectively.

Our earlier treatment has shown us how to generalize this to $t_0 \neq 0$.

Constructing the solution the standard way: In the standard treatment, using $a = \omega^2$, the general solution still reads

$$q(t) = A_1 e^{(-\gamma+\sqrt{\gamma^2-\omega^2})t} + A_2 e^{(-\gamma-\sqrt{\gamma^2-\omega^2})t} \tag{1.8.30}$$

provided $\omega \neq \gamma$. At $\omega = \gamma$ one finds instead that

$$q(t) = A_1 e^{-\gamma t} + A_2 t e^{-\gamma t} \tag{1.8.31}$$

In all cases, the overall exponential decay factor $e^{-\gamma t}$ will, eventually, bring all motion to a standstill, no matter the value of ω.

The "oscillatory" factors, themselves are affected by the presence of γ and show decidedly different behavior depending of the value of ω i.e. the curvature of the potential $U(q) = \frac{m}{2}\omega^2 q^2$.

› **$\omega^2 > \gamma^2$, underdamped oscillations:** Here $\sqrt{\gamma^2 - \omega^2} =: i\tilde{\omega}$ with $\tilde{\omega}$ real leads to damped oscillations:

$$e^{\pm\sqrt{\gamma^2-\omega^2})t} = e^{\pm i\tilde{\omega}t} \tag{1.8.32}$$

$\tilde{\omega}$ is a modified oscillation frequency

- $\omega^2 < \gamma^2$**, overdamped oscillation :** Here $\sqrt{\gamma^2-\omega^2} = \tilde{\gamma}$ is real so that no oscillations occur at all. Note that $\gamma > \tilde{\gamma} = \sqrt{\gamma^2-\omega^2}$ in this case, both terms

$$e^{-(\gamma \pm \sqrt{\gamma^2-\omega^2})t} = e^{-(\gamma\pm\tilde{\gamma})t} \tag{1.8.33}$$

  decay (there are no runaway solutions).

- $\omega^2 = \gamma^2$**, critical damping:** this is the "fastest moving" case for which there is no oscillation and is hence termed *critical damping*. One may solve this using the basis set for degenerate solution, but we will proceed differently, see below.

Let us complete our solution by determining the A_i in terms of initial coordinates and momenta at $t_0 = 0$, starting with the underdamped case. The general solution reads

$$q(t) = e^{-\gamma t}(A_1 + A_2)\cos(\sqrt{\omega^2-\gamma^2}t) - i(A_1 - A_2)\sin(\sqrt{\omega^2-\gamma^2}t) \tag{1.8.34}$$

so that initial conditions at $t_0 = 0$ in terms of $q(0)$ and $p(0)$ require

$$q(t_0=0) \stackrel{!}{=} A_1 + A_1 \; ; \qquad p(t_0=0) = m\dot{q}(t=t_0) \stackrel{!}{=} m\big(-i\sqrt{\omega^2-\gamma^2}(A_1-A_2) - \gamma(A_1+A_2)\big) \tag{1.8.35}$$

with the solutions

$$A_1 + A_2 = q(t_0=0) \qquad A_1 - A_2 = i\left(p(t_0=0)\frac{1}{m\sqrt{\omega^2-\gamma^2}} + q(t_0=0)\frac{\gamma}{m\sqrt{\omega^2-\gamma^2}}\right) \tag{1.8.36}$$

The solution comes out to be real with units of length and of the form

$$\begin{aligned} q(t) = e^{-\gamma(t-t_0)}\Bigg[&\left(\cos(\sqrt{\omega^2-\gamma^2}(t-t_0)) + \frac{\gamma\sin(\sqrt{\omega^2-\gamma^2}(t-t_0))}{\sqrt{\omega^2-\gamma^2}}\right)q(t_0) \\ &+ \frac{\sin(\sqrt{\omega^2-\gamma^2}(t-t_0))}{m\sqrt{\omega^2-\gamma^2}}p(t_0)\Bigg] \end{aligned} \tag{1.8.37}$$

Once expressed in terms of physical initial conditions $q(t_0)$ and $p(t_0)$, we may in fact lift any restrictions on γ vs ω: Taking the limit $\gamma \to \omega$ we immediately obtain

$$q(t) = e^{-\gamma(t-t_0)}\left[q(t_0)\,(1+\gamma(t-t_0)) + \frac{p(t_0)}{m}(t-t_0)\right] \tag{1.8.38}$$

which is precisely of the form (1.8.24).

Also the overdamped solution at $\gamma > \omega$ is recovered, by simply replacing $\sqrt{\omega^2-\gamma^2} \to i\sqrt{\gamma^2-\omega^2} =: i\tilde{\gamma}$ and noting that $\cos(ix) = \cosh(x)$, $\sin(ix) = i\sinh(x)$. After recasting the trigonometric functions as exponentials one obtains

$$q(t) = \frac{q(t_0)}{2\tilde{\gamma}}\left((\tilde{\gamma}-\gamma)e^{-(\gamma-\tilde{\gamma})(t-t_0)} + (\tilde{\gamma}+\gamma)e^{-(\gamma+\tilde{\gamma})(t-t_0)}\right) + \frac{p(t_0)}{2m\tilde{\gamma}}\left(e^{-(\gamma-\tilde{\gamma})(t-t_0)} + e^{-(\gamma+\tilde{\gamma})(t-t_0)}\right) \tag{1.8.39}$$

physical and mathematical pendulum, constraints, tension of rod

1.8.3 Example: the pendulum, spherical and planar, mathematical and physical

In the previous two sections we have discussed the harmonic oscillator as a rather abstract mathematical device: we have not tied it to a physical realization.

I will now move towards a more physical system by considering a "spherical pendulum" and then consider a number of special cases and approximations.

A spherical pendulum consists of a point mass m moving without friction on the surface of a two dimensional sphere of some radius R in a uniform gravitational field, exerting a gravitational force of the form $m\boldsymbol{g}$ with $\boldsymbol{g} = -g\hat{\boldsymbol{z}}$ directed "downwards".

Of course in a physical realization we need a "device" that keeps the mass on the surface of the sphere, and therein lies the problem: One may realize this with a gimbal[4], but it appears to be a formidable task to make its mass irrelevant without endangering mechanical stability.

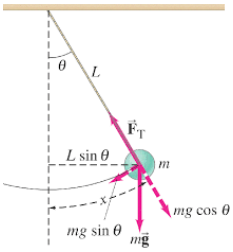
Easier to realize is the mathematical pendulum: This is a device in which a (ideally massless) mass m can rotate on a circle in a vertical plane. We can approximate that with mass at the end of a rod suspended at a right angle from a horizontal axis that can rotate with little friction.

First, however, let us deal with the abstract mathematical problem.

The condition that the mass remains on the sphere or a vertical circle is usually referred to as a constraint. Since gravity would automatically pull the mass away from the spherical surface, the device keeping the mass on the sphere or circle must exert a force. In physical realizations in which a stiff rod provides the means one speaks of "tension" and tension forces. More generally we speak of a constraint force.

For the problem at hand it is easiest to describe this in spherical coordinates in which we place the north pole in the negative z direction, i.e. we rotate the coordinate system around $\boldsymbol{y}$ by π, so that $\eta = \theta + \pi$ describes counterclockwise deviations from the stable configuration with the mass at rest at the lowest point of the sphere.

$$\boldsymbol{r} = -r \begin{pmatrix} \cos\phi \sin\eta \\ \sin\phi \sin\eta \\ \cos\eta \end{pmatrix} \tag{1.8.40}$$



The forces acting in the problem are the gravitational force The the rod suspended from above exerts a tension force $\boldsymbol{T}$ that that prevents the mass from going into free fall. It acts purely in a radial direction and simply balances the radial component of the gravitational force to prevent radial movement. The geometry of this is depicted int fig:

$$\boldsymbol{T} = -mg\cos(\eta)\boldsymbol{e}_r \tag{1.8.41}$$

[4] "Kardanische Aufhängung" for the Germans among tou.

and the remaining force

$$m\boldsymbol{g} - mg\cos(\eta)\boldsymbol{e}_r = -mg\sin(\eta)\boldsymbol{e}_\eta \tag{1.8.42}$$

is parallel to $\boldsymbol{e}_\eta$.

The trajectories can be expressed entirely in terms of $\boldsymbol{e}_\eta$ and $\boldsymbol{e}_\phi$

A solution of the mathematical pendulum at arbitrary extensions can be given in terms of Jacobi functions. See[4] for a derivation. The result is:

$$\theta(t) = 2\arcsin\Big(\sin(\theta_0/2)\ \mathrm{sn}\big[K(\sin^2(\theta_0/2) - \omega_0 t; \sin^2(\theta_0/2)\big]\Big) \tag{1.8.43}$$

The planar mathematical pendulum provides a somewhat more sophisticated example for the phase space structure. Clearly this system will have two equilibrium points:

- A *stable equilibrium* with $U'' > 0$ (the pendulum hanging down)
- An *unstable equilibrium* point with $U'' < 0$(the pendulum standing upright)

Fix Graphics

Strictly speaking, the planar pendulum is already a constrained system: a mass point moves on a circle of constant radius, as sketched in Fig. 3

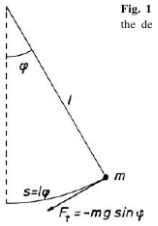


Fig. 3: *planar pendulum*

However, it is so simple that we may treat it like a free one-dimensional system and do not need the full formalism of constrained motion yet. We denote by $\varphi(t)$ the angle that measures the deviation of the pendulum from the vertical and by $s(t) = l\varphi(t)$ the length of the corresponding arc on the circle. We then have

$$T = \frac{1}{2}m\dot{s}^2 = \frac{1}{2}ml^2\dot{\varphi}^2 \tag{1.8.44}$$

$$U = \int_0^s ds' mg\sin(\varphi(s')) = mgl\int_0^\varphi d\varphi'\ \sin(\varphi') = -mgl[\cos\varphi - 1] \tag{1.8.45}$$

Energy is the only conserved quantity, and we choose dimensionless variables to characterize the system in a generic manner:

$$\epsilon := \frac{E}{mgl} = \frac{\dot{\varphi}^2}{2\omega^2} + 1 - \cos\varphi \qquad \text{where} \qquad \omega^2 := \frac{g}{l} \tag{1.8.46}$$

Similarly to what we have done for the harmonic oscillator, we set $z_1 = \varphi$, $\tau = \omega t$, and $z_2 = \dot{\varphi}/\omega$. Then

$$\epsilon = \underbrace{z_2^2/2}_{T} + \underbrace{1 - \cos z_1}_{U} \tag{1.8.47}$$

while

$$\frac{d}{d\tau}\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} z_2(\tau) \\ -\sin(z_1(\tau)) \end{pmatrix} . \tag{1.8.48}$$

In the limit of small deviations from the vertical one has $\sin z_1 = z_1 + O(z_1^3)$ and Eq. (1.8.48) reduces to the system of the oscillator.

The general solution to Eq. (1.8.48) is no longer as simple as before, (instead of $\boldsymbol{z}^2$ it is $z_2^2/2 + 1 - \cos z_1$ that must be preserved by the flow map Φ_{τ,τ_0}, if such a thing exists) but some general features remain which we will now turn to:

Fix Graphics

In Fig. 4 we sketch the potential $U(z_1)$ and some phase portraits. For values of ϵ below 2 the picture is qualitatively similar to that of the oscillator. The smaller ϵ, the closer the similarity. We distinguish several

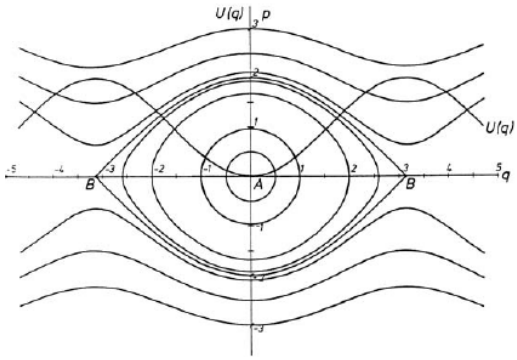


Fig. 4: *Phase portrait and potential of the planar pendulum. A: Stable equilibrium at bottom, B: unstable equilibrium at top of rotation.*

types of phase space trajectories:

- $\epsilon > 2$: the pendulum has enough kinetic energy to keep rotating through the unstable upright position (either to the left or to the right, represented by the "wavy" orbits at the top and bottom respectively)
- $\epsilon < 2$: periodic orbits in which the pendulum swings back and forth
- $\epsilon = 2$: The *separatrix* (of the two previous cases) in which the system if starting anywhere away from the unstable equilibria at B moves towards B but takes infinite time to reach it.
- the equilibria at A and B are separate point like trajectories – without external perturbations, the system stays stationary at these points.

Note again that none of these orbits cross: a single point on one of the orbits is sufficient to uniquely tag the orbit as a whole and thus to completely predict the behavior of the system at all times.

1.9 Existence and uniqueness of solutions, local flow in phase space

The features encountered in the two examples above are in fact prototypical: at least locally, near some initial condition all of the features discussed above remain true of the solutions of

$$\dot{\boldsymbol{x}} = \boldsymbol{F}(x,t) \ , \tag{1.9.1}$$

a single point $\boldsymbol{x}_0 \in \mathsf{P}$ together with Eq. (1.9.1) selects one orbit in the whole phase space trajectory portrait. This point $\boldsymbol{x}_0$, which defines the positions and momenta (or velocities), can be understood as the initial condition that is assumed at a given time $t = t_0$. This condition defines how the system will continue to evolve locally. The theory of ordinary differential equations gives precise information about the existence and uniqueness of solutions for (1.9.1), provided the function $\boldsymbol{F}(\boldsymbol{x},t)$ fulfills certain conditions. This information is of immediate relevance for physical orbits that are described by Newton's equations. We quote the following basic theorem but refer to the literature for its proof (see e.g. Arnol'd textbooks on differential equations [5, 6]).

› **Theorem 1 – Uniqueness and existence of solutions to first order differential equations:**
Let $\boldsymbol{F}(\boldsymbol{x},t) \neq 0$ with $\boldsymbol{x} \in \mathbb{P}$ and $t \in \mathbb{R}$ be continuous and, with respect to $\boldsymbol{x}$, continuously differentiable. Then, for any $\boldsymbol{z} \in \mathbb{P}$ and any $t_0 \in \mathbb{R}$ a neighborhood U of $\boldsymbol{x}_0$ and an open interval I around t_0 such that for all $x_0 \in U$ there is precisely one curve $\boldsymbol{x}(t,t_0,\boldsymbol{x}_0)$ with $t \in I$ that fulfills the following conditions:

$$\frac{\partial}{\partial t}\boldsymbol{x}(t,t_0,\boldsymbol{x}_0) = \boldsymbol{F}(\boldsymbol{x}(t,t_0,\boldsymbol{x}_0),t) \tag{1.9.2a}$$

$$x(t_0,t_0,\boldsymbol{x}_0) = \boldsymbol{x}_0 \tag{1.9.2b}$$

$$x(t,t_0,\boldsymbol{x}_0) \ \text{ has continuous derivatives in } t,\ t_0, \text{ and } \boldsymbol{x}_0 \tag{1.9.2c}$$

$\boldsymbol{x}_0$ is the initial point in phase space from which the system starts at time $t = t_0$. The solution $\boldsymbol{x}(t,t_0,\boldsymbol{x}_0)$ is called the integral curve of the vector field $\boldsymbol{F}(\boldsymbol{x},t)$.

This has a number of immediate and general consequences for systems described by the equations of motion $\dot{\boldsymbol{x}} = \boldsymbol{F}(\boldsymbol{x},t)$:

- They are finite dimensional, i.e. every state of the system is completely determined by a point $\boldsymbol{x}_0 \in \mathbb{P}$. The phase space has dimension $6n = 2f$, where f is the number of degrees of freedom.
- They are deterministic, i.e. the initial positions and momenta determine the solution locally (depending on the maximal neighborhood U and maximal interval I) in a unique way. In particular, this means that two phase curves do not intersect (in U and I).

If we know all solutions corresponding to all possible initial conditions $\boldsymbol{x}(t,t_0,\boldsymbol{x}_0)$ we may interpret this as the result of a map

$$\boldsymbol{x}(t,s,\boldsymbol{y}) =: \Phi_{t,s}(\boldsymbol{y}) \tag{1.9.3}$$

$$\Phi_{t,s} : \mathbb{P} \to \mathbb{P} \tag{1.9.4}$$

$$\boldsymbol{y} \mapsto \boldsymbol{x} \tag{1.9.5}$$

called the flow in phase space. The theorem above assures us that this map is unique and both it and its inverse are differentiable. With the times $r, s, t \in I$ we then have

$$\Phi_{t,s} \circ \Phi_{s,r} = \Phi_{t,r} \qquad \Phi_{t,s}^{-1} = \Phi_{s,t} \qquad \Phi_{s,s} = 1$$
$$\frac{\partial}{\partial t}\Phi_{ts} = F_t \circ \Phi_{ts} \qquad F_t := \frac{\partial}{\partial t}\Phi_{ts}\Big|_{s=t} \tag{1.9.6}$$

This ensures that the Φ form what is known as one parameter groups.

For *autonomous* systems –systems where F_t is independent of time $\Phi_{t,s} = \Phi_{t-s}$. Such systems are invariant under time translations.

The two examples, the harmonic oscillator, and the planar mathematical pendulum, match perfectly with these statements:

- For the harmonic oscillator, we had already anticipated the notation

$$\Phi_{t-t_0} = e^{-(\tau-\tau_0)J} = \begin{pmatrix} \cos(\tau-\tau_0) & \sin(\tau-\tau_0) \\ -\sin(\tau-\tau_0) & \cos(\tau-\tau_0) \end{pmatrix} \tag{1.9.7}$$

  This is a direct example that the flow Φ forms a one parameter group of maps on phase space: the properties in Eq. (1.9.6) are immediately verified.

  We note in addition that the origin of the phase space portrait is special: it corresponds to an orbit that consists of a single point. Note that this does not contradict theorem 1.

- For the pendulum it is not so easy to write down Φ, but the theorem assures at that it exists on open sets $U \in \mathbb{P}$ for open intervals $I \in \mathbb{R}$ – this latter property is important for the separatrix. Why?

1.10 Linear systems and linear approximations

Of the examples for dynamical systems we have encountered above, the harmonic oscillator provides the prime example for a linear system, a system where the phase space equations of motions become

$$\dot{\boldsymbol{x}} = A\boldsymbol{x} + \boldsymbol{b} \tag{1.10.1}$$

where A is a linear map on phase space and $\boldsymbol{b}$ is a vector in phase space. Both A and $\boldsymbol{b}$ may be time dependent.

As is customary, we call the equation that emerges from Eq. (1.10.1) by setting $\boldsymbol{b}$ to $\boldsymbol{0}$ the associated homogeneous equation. Eq. (1.10.1) is accordingly called the inhomogeneous equation.

The crucial observation is that any two solutions of the inhomogeneous system differ by a solution of the homogeneous equation. Thus a general solution to the inhomogeneous equation can always be written as a general solution to the homogeneous system plus an *arbitrary* solution to the inhomogeneous problem.

Comparing with Eq. (1.8.18),

$$\frac{d}{dt}\begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} 0 & \frac{1}{m} \\ -m\omega^2 & -2\gamma \end{pmatrix}\begin{pmatrix} q \\ p \end{pmatrix}$$

for the damped harmonic oscillator reveals that in this case

$$A = \begin{pmatrix} 0 & \frac{1}{m} \\ -m\omega^2 & -2\gamma \end{pmatrix} \tag{1.10.2}$$

is time independent and $\boldsymbol{b}$ is outright zero. A simple, but physically relevant modification arises if we subject the system to a periodic external forcing term...

1.10.1 The forced harmonic oscillator

We return to the equation of motion of a single harmonic oscillator

$$m\ddot{q} + 2m\gamma\dot{q} + kq = F(t) \qquad \text{or} \qquad \ddot{q} + \frac{2}{\gamma}\dot{q} + \omega^2 q = \frac{1}{m}F(t) \tag{1.10.3}$$

$\tau := \frac{1}{\gamma}$ is called the relaxation time (indeed it must have dimension [time]) and ω_0 is the frequency of the undamped oscillation and carries $[\omega_0] = [\text{time}]^{-1}$.

A very general method to find a solution to Eq. (1.10.3) employs Green's functions $G(t-t')$.

Any function $G(t-t')$ that satisfies

$$\ddot{G}(t-t') + 2\gamma\dot{G}(t-t') + \omega^2 G(t-t') = \delta(t-t') \tag{1.10.4}$$

allows us to write a solution to Eq. (1.10.3) in the form

$$q(t) = \frac{1}{m}\int_{-\infty}^{\infty} dt\; G(t-t')F(t') \tag{1.10.5}$$

since

$$\begin{aligned}\ddot{q}(t) + 2\gamma\dot{q}(t) + \omega^2 q(t) &= \int_{-\infty}^{\infty} dt\; \Big(\ddot{G}(t-t') + 2\gamma\dot{G}(t-t') + \omega^2 G(t-t')\Big)F(t') \\ &= \frac{1}{m}\int_{-\infty}^{\infty} dt\; \delta(t-t')F(t') = \frac{1}{m}F(t)\end{aligned} \tag{1.10.6}$$

We note that the defining equation looks like our original equation for $q(t)$ if for a very specific forcing term. As such it has many solutions: Eq. (1.10.4) determines G only up to arbitrary solutions of the corresponding homogeneous equation. Since we have already found all solutions to the homogeneous equation, we will be be content to find one specific solution. It is surprisingly easy to do so using Fourier transforms for both G and the δ-distribution:

$$G(t-t') = \int_{-\infty}^{\infty} \frac{d\tilde{\omega}}{2\pi} e^{i\tilde{\omega}(t-t')} G(\tilde{\omega}) \qquad \text{and} \qquad \delta(t-t') = \int_{-\infty}^{\infty} \frac{d\tilde{\omega}}{2\pi} e^{i\tilde{\omega}(t-t')} \tag{1.10.7}$$

Eq. (1.10.4) then becomes surprisingly simple

$$\int_{-\infty}^{\infty} \frac{d\tilde{\omega}}{2\pi} e^{i\tilde{\omega}(t-t')} \left(-\tilde{\omega}^2 + i2\gamma\tilde{\omega} + \omega^2\right) G(\tilde{\omega}) \stackrel{!}{=} \int_{-\infty}^{\infty} \frac{d\tilde{\omega}}{2\pi} e^{i\tilde{\omega}(t-t')} \tag{1.10.8}$$

so that we obtain

$$G(t-t') = \int_{-\infty}^{\infty} \frac{d\tilde{\omega}}{2\pi} \frac{e^{i\tilde{\omega}(t-t')}}{-\tilde{\omega}^2 + i2\gamma\tilde{\omega} + \omega^2} \tag{1.10.9}$$

Despite superficial appearances $G(t-t)$ is real: taking its complex conjugate we only need to change integration variable, from $\tilde{\omega}$ to $-\tilde{\omega}$, to recover the original expression. As a consequence, a real forcing term $F(t)$ will always produce a real response through Eq. (1.10.5).

As discussed, this corresponds to one of infinitely many possible solutions to the inhomogeneous equation (1.10.4). Any such pair of solutions differs by the initial conditions it satisfies. The specific initial conditions satisfied by the solution above can only be discerned after we carry out the Fourier transformation in Eq. (1.10.9).

This can be easily done using a little complex analysis and Cauchy's theorem.

We observe that the integrand has poles in the complex plane at

$$\tilde{\omega}_\pm = i\gamma \pm \sqrt{\omega^2 - \gamma^2} \tag{1.10.10}$$

So that

$$G(t-t') = \int_{-\infty}^{\infty} \frac{d\tilde{\omega}}{2\pi} \frac{e^{i\tilde{\omega}(t-t')}}{-(\tilde{\omega}-\tilde{\omega}_+)(\tilde{\omega}-\tilde{\omega}_-)} \tag{1.10.11}$$

The key idea on performing the $\tilde{\omega}$ integral along the real axis is to view it as part of a complex countour integral along a closed contour in which the contribution from the closing part (away from the real axis) vanishes. Imagine we add a half circle at infinity, either in the upper or in the lower half plane as sketched in Fig. 5. The integrand reads

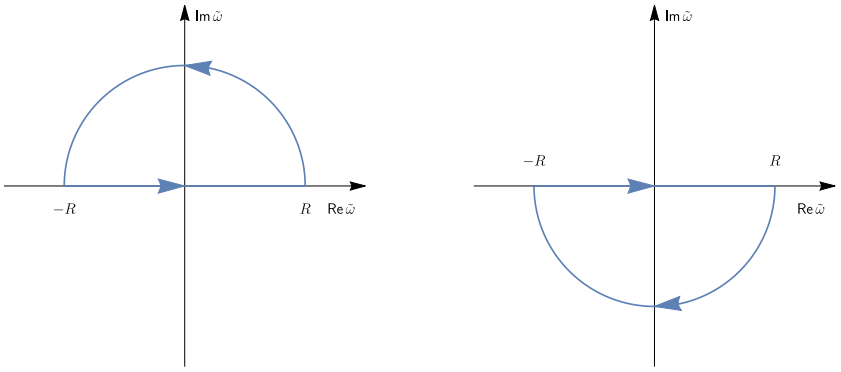


Fig. 5: *Integration contours along the real axis amended with arcs in either the lower or upper half plane. Of interest to us is the limit $R \to \infty$ where the half circles are pushed away to infinity.*

$$\frac{e^{i\tilde{\omega}(t-t')}}{-(\tilde{\omega}-\tilde{\omega}_+)(\tilde{\omega}-\tilde{\omega}_-)} = \frac{e^{i\mathsf{Re}\tilde{\omega}(t-t')-\mathsf{Im}\tilde{\omega}(t-t')}}{-(\tilde{\omega}-\tilde{\omega}_+)(\tilde{\omega}-\tilde{\omega}_-)} \tag{1.10.12}$$

and one must understand its behavior on the arc as it moves out to infinity with $R \to \infty$. Near the real axis the denominator falls of as $1/\tilde{\omega}^2$ and suppresses all contributions to the integral. As we move away from the real axis the exponential factor $e^{-\mathsf{Im}\tilde{\omega}(t-t')}$ either diverges or leads to zero depending on the sign of the exponent. When divergence occurs the amended integral also becomes infinite and will not be of use. Convergence occurs when

$$\mathsf{Im}\tilde{\omega} > 0 \text{ and } (t-t') > 0 \text{ This corresponds to closing the contour in the upper half plane.} \tag{1.10.13}$$

$$\mathsf{Im}\tilde{\omega} < 0 \text{ and } (t-t') < 0 \text{ This corresponds to closing the contour in the upper lower plane.} \tag{1.10.14}$$

In both cases the arc at infity does not contribute to the integral. Thus we may write

$$\begin{aligned} G(t-t') &= \int_{-\infty}^{\infty} \frac{d\tilde{\omega}}{2\pi} \frac{e^{i\tilde{\omega}(t-t')}}{-(\tilde{\omega}-\tilde{\omega}_+)(\tilde{\omega}-\tilde{\omega}_-)} \\ &= \theta(t-t') \int_{\frown} \frac{d\tilde{\omega}}{2\pi} \frac{e^{i\tilde{\omega}(t-t')}}{-(\tilde{\omega}-\tilde{\omega}_+)(\tilde{\omega}-\tilde{\omega}_-)} + \theta(t'-t) \int_{\smile} \frac{d\tilde{\omega}}{2\pi} \frac{e^{i\tilde{\omega}(t-t')}}{-(\tilde{\omega}-\tilde{\omega}_+)(\tilde{\omega}-\tilde{\omega}_-)} \end{aligned} \tag{1.10.15}$$

with the θ-functions taking care of the case distinction.

Both terms are now integrals along closed contours, with integrands that contain only poles. These can be evaluated using residues. One finds

$$G(t-t') = \theta(t-t') 2\pi i \underset{\frown}{\mathsf{Res}} \left(\frac{1}{2\pi} \frac{e^{i\tilde{\omega}(t-t')}}{-(\tilde{\omega}-\tilde{\omega}_+)(\tilde{\omega}-\tilde{\omega}_-)} \right) - \theta(t'-t) 2\pi i \underset{\smile}{\mathsf{Res}} \left(\frac{1}{2\pi} \frac{e^{i\tilde{\omega}(t-t')}}{-(\tilde{\omega}-\tilde{\omega}_+)(\tilde{\omega}-\tilde{\omega}_-)} \right) \tag{1.10.16}$$

where the minus sign in the second term arises due to the clockwise orientation of the contour.

We need to distinguish three cases as before and determine where $\tilde{\omega}_\pm = i\gamma \pm \sqrt{\omega^2-\gamma^2}$ places the poles. Since $\gamma \geq 0$ and the eigen value ω is real (this is not affected by considering complex values for the integration variable $\tilde{\omega}$) we face:

- **The underdamped case** $\omega > \gamma$**:** We encounter two single poles, both in the upper half plane.
- **The critically damped case** $\omega = \gamma$**:** we encounter a double pole in the upper half plane.
- **The overdamped case** $\omega_0 < \gamma$**:** We encounter two single poles on the imaginary axis, both in the upper half plane.

Note that in all cases the poles are strictly in the upper half plane so that the second term will not contribute in any of the three cases.

In the following I will only discuss the underdamped case. One obtains

$$\begin{aligned} G(t-t') &= -i\theta(t-t') \left(\frac{e^{i\omega_+(t-t')}}{\omega_+-\omega_-} + \frac{e^{i\omega_-(t-t')}}{\omega_--\omega_+} \right) \\ &= \theta(t-t') \frac{e^{-\gamma(t-t')}}{\sqrt{\omega^2-\gamma^2}} \frac{1}{2i} \left(e^{i\sqrt{\omega^2-\gamma^2}(t-t')} - e^{-i\sqrt{\omega^2-\gamma^2}(t-t')} \right) \end{aligned} \tag{1.10.17}$$

This result is surprisingly simple, one arrives at

$$G(t-t') = \theta(t-t') e^{-\gamma(t-t')} \frac{\sin\left(\sqrt{\omega^2-\gamma^2}(t-t')\right)}{\sqrt{\omega^2-\gamma^2}} \tag{1.10.18}$$

This result has substructure that is worth exposing.

By comparing with Eq. (1.8.37) we verify that the function

$$P(t-t') = e^{-\gamma(t-t')} \frac{\sin\left(\sqrt{\omega^2-\gamma^2}(t-t')\right)}{\sqrt{\omega^2-\gamma^2}} \tag{1.10.19}$$

is a solution to the homogeneous equation with boundary conditions

$$P(0) = 0 \qquad \dot{P}(0) = 1 \tag{1.10.20}$$

The factor $\theta(t-t')$ in Eq. (1.10.18) encodes causality: The contributions of any forcing in Eq. (1.10.5) at time t' only affects the solution at times t later that t'.

We observe that P does not only apper as part of the Green's function, it also plays a prominent role in our expressions for the general solution of the harmonic oscillator equation in the absence of a driving force, Eq. (1.8.37):

$$\begin{aligned} q(t) &= e^{-\gamma(t-t_0)}\left[q(t_0)\left(\cos(\sqrt{\omega^2-\gamma^2}(t-t_0)) + \frac{\gamma\sin(\sqrt{\omega^2-\gamma^2}(t-t_0))}{\sqrt{\omega^2-\gamma^2}}\right)\right. \\ &\qquad \left. + p(t_0)\frac{\sin(\sqrt{\omega^2-\gamma^2}(t-t_0))}{m\sqrt{\omega^2-\gamma^2}}\right] \\ &= (\frac{d}{dt}+\gamma)P(t-t_0)q(t_0) + P(t-t_0)\left(\frac{d}{dt}q\right)(t_0)\ . \end{aligned} \tag{1.10.21}$$

Eq. (1.10.21) states that we can use P and its derivatives to "propagate" the initial conditions $q(t_0)$ and $\dot{q}(t_0)$ at t_0 to any other time t. For this reason P is generally called the *propagator* of the harmonic oscillator.

› **Remark 1.10 – consistency check for the $G(t-t')$:**

Can we see directly, without a detour through Fourier space, that $G(t-t')$ satisfies its defining equation (1.10.4)? Let's see:

$$\begin{aligned} \ddot{G}(t-t') &+ 2\gamma\dot{G}(t-t') + \omega_0^2 G(t-t') \\ &= \ddot{\theta}(t-t')P(t-t') + 2\dot{\theta}(t-t')\dot{P}(t-t') + \theta(t-t')\ddot{P}(t-t') \\ &\quad + 2\gamma\Big(\dot{\theta}(t-t')P(t-t') + \theta(t-t')\dot{P}(t-t')\Big) \\ &\quad + \omega_0^2\theta(t-t')P(t-t') \end{aligned}$$

The terms proportional to the undifferentiated θ functions sum to zero since P satisfies the homogeneous equation. Using $\dot{\theta}(t-t) = \delta(t-t')$ on the remaining terms, this leaves us with

$$= \dot{\delta}(t-t')P(t-t') + \delta(t-t')\Big(2\dot{P}(t-t') + 2\gamma P(t-t')\Big)$$

The $\dot{\delta}$ terms would appear to be dangerous, but the expression can be rearranged to demonstrate that all is well overall. To this end, we note that the distribution $\frac{d}{dt}(\delta(t-t')P(t-t'))$ is far from undefined – it equals the zero distribution on all test functions, since $P(0) = 0$ (partial integration). Rearranging terms using $\dot{\theta}(t-t')P(t-t') = \frac{d}{dt}(\delta(t-t')P(t-t')) - \theta(t-t')\dot{P}(t-t')$ splits the suspicious term into two well defined distributions and leads to

$$\begin{aligned} &= \frac{d}{dt}\Big(\delta(t-t')P(t-t')\Big) + \delta(t-t')\Big(\dot{P}(t-t') + 2\gamma P(t-t')\Big) \\ &= \delta(t-t') \end{aligned} \tag{1.10.22}$$

The last step follows using the initial conditions for $P(t-t)$.

› **Remark 1.11 – resonance:**

Given that the eigenstates of the harmonic oscillator are harmonic functions, it should not come as a surprise that a harmonic forcing term of the form

$$F_\Omega(t) := mf\sin(\Omega t) \tag{1.10.23}$$

leads to particularly simple responses.

$$\begin{aligned} q(t) &= \frac{1}{m}\int_{-\infty}^{\infty} dt'\; G(t-t')F_\Omega(t') \\ &= f\int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\frac{e^{i\omega(t-t')}}{-\omega^2+i2\gamma\omega+\omega_0^2}\frac{1}{2i}\left(e^{i\Omega t'}-e^{-i\Omega t'}\right) \end{aligned} \tag{1.10.24}$$

We recognize Frouier representations of the δ distributions:

$$\int_{-\infty}^{\infty} dt' e^{i(\omega\pm\Omega)t'} = 2\pi\delta(\omega\pm\Omega) \tag{1.10.25}$$

so that

$$\begin{aligned} q(t) &= f\int_{-\infty}^{\infty} d\omega\; \frac{e^{i\omega t}}{-\omega^2+i2\gamma\omega+\omega_0^2}\frac{1}{2i}\left(\delta(\omega+\Omega)-\delta(\omega-\Omega)\right) \\ &= \frac{f}{2i}\left(\frac{e^{-i\Omega t}}{-\Omega^2-2i\gamma\Omega+\omega^2}-\frac{e^{+i\Omega t}}{-\Omega^2+2i\gamma\Omega+\omega^2}\right) \\ &= \frac{f}{(\Omega^2-\omega^2)^2+(2\gamma\Omega)^2}\left((\Omega^2-\omega^2)\sin(\Omega t)+2\gamma\Omega\cos(\Omega t)\right) \end{aligned} \tag{1.10.26}$$

The result is reassuringly real (as it has to be since both G and the force are).

We note that in the damped case, this is the solution the system approches at large times, since the homogeneous solution we can add to this will eventually decay.

To fully appreciate its behavior it helps tremendously to recast it in terms of single harmonic function (instead of the linear combination appearing above). This way we can identify a single amplidude that governs the size of the response and a phase shift that governs the relative lag between force and response.

To this end, we note that the coefficients of the $\sin(\Omega t)$ and $\cos(\Omega t)$ in the bracketed expression can be rewritten in terms of the components of a two component unit vector and a prefactor that restores the

length according to

$$a\sin(\alpha) + b\cos(\alpha) = \sqrt{a^2+b^2}\left(\frac{a}{\sqrt{a^2+b^2}}\sin(\alpha) + \frac{b}{\sqrt{a^2+b^2}}\cos(\alpha)\right) \tag{1.10.27}$$

The normalized coefficients can then be interpreted as the sin and cos of an angle. We set

$$\frac{a}{\sqrt{a^2+b^2}} =: \sin(\phi) \qquad \text{and consistently} \qquad \frac{b}{\sqrt{a^2+b^2}} = \cos(\phi) \tag{1.10.28}$$

and use $\cos(\phi)\sin(\alpha) + \sin(\phi)\cos(\alpha) = \sin(\alpha+\phi)$ to combine the sum of oscillating functions into a single one, phase shifted by ϕ:

$$q(t) = \frac{1}{\sqrt{(\Omega^2-\omega^2)^2 + (2\gamma\Omega)^2}}\sin(\Omega t + \phi) \tag{1.10.29}$$

where

$$\tan(\phi) = \frac{2\gamma\Omega}{\omega^2-\Omega^2} \qquad \text{i.e.} \qquad \phi(\Omega) = \arctan\left(\frac{2\gamma\Omega}{\omega^2-\Omega^2}\right) + \theta(\Omega-\omega)\pi \tag{1.10.30}$$

The strongest response occurs where the amplitude

$$A(\Omega) := \frac{1}{\sqrt{(\omega^2-\Omega^2)^2 + (2\gamma\Omega)^2}} \tag{1.10.31}$$

has its maximum. This occurs at the resonance frequency

$$\Omega_r = \sqrt{\omega^2 - 2\gamma^2} \tag{1.10.32}$$

For $\Omega \ll \omega$ the response is almost in phase with the forcing. In the opposite limite that $\Omega \gg \omega$ the phase shift becomes maximal, $\phi \to \pi$. For $\Omega = \omega$ the phase shift is precisely $\pi/2$. This behavior is shown in Fig. 6.

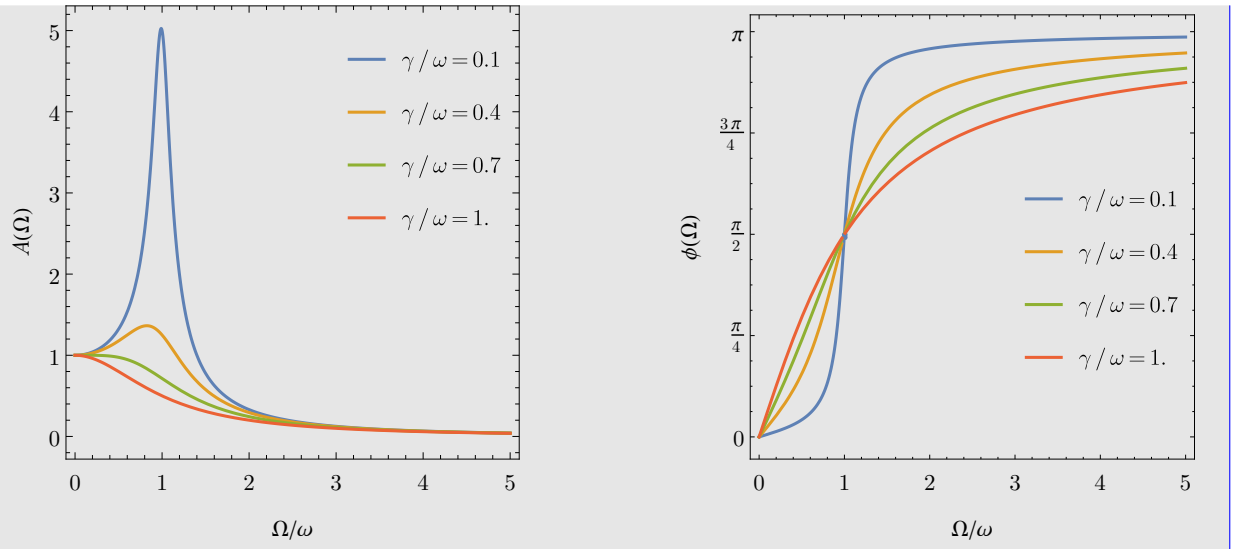


Fig. 6: *Amplitude (left) and phase (right) of the damped, forced harmonic oscillator at large times. The resonance phenomenon, with a maximum in the amplitude, becomes visible only at small enough γ. Below $\gamma/\omega < 1/\sqrt{2}$ a maxium forms and becomes more and more pronouced as we lower damping coefficient even further.*



12 – perturbation theory for an anharmonic oscillator:

This whole section is



1.11 Coupled oscillators

We will describe our system with a set of generalized coordinates q_i which we collectively denote $\boldsymbol{q}$ (but beware: they need not live in a vector space).

We restrict ourselves to systems that are conservative, that is they possess a potential energy $V(\boldsymbol{q})$. In addition we assume that the system is stable, i.e. that the potential posesses at least local minima and denote the one of interest by $\boldsymbol{q}_0$.

We assumme the system to be near that minimum and will only attempt to learn about small disturbances in the vicinity of that minimum. For simplicity we adapt coordinates such that $\boldsymbol{q}_0 = \boldsymbol{0}$. This allows us to Taylor expand:

$$V(\boldsymbol{q}) = V(\boldsymbol{0}) + \frac{\partial V}{\partial q_i}(\boldsymbol{0})q_i + \frac{1}{2}\frac{\partial^2 V}{\partial q_i \partial q_j}(\boldsymbol{0})q_i q_j + \mathcal{O}(q^3) \tag{1.11.1}$$

In this expansion the constant term is irrelevant (a potential energy is only defined up to an overall constant) and the linear term vanishes since $\boldsymbol{q}_0$ is an extremum.

The kinetic term is of the form

$$T = T_{ij}\dot{q}_i\dot{q}_j \tag{1.11.2}$$

with T_{ij} symmetric in its indices.

The equations of motion become

$$T_{ij}\ddot{q}_j + V_{ij}q_j = 0 \tag{1.11.3}$$

and can be turned into a set of algebraic equations by Fourier transforming in time, since any stationary solution to Eq. (1.11.3) is of the form

$$\boldsymbol{a}_+ e^{i\omega t} + \boldsymbol{a}_- e^{-i\omega t} \tag{1.11.4}$$

Inserting the linearly indpendent terms into Eq. (1.11.3) leads to

$$(-T\omega^2 + V)\boldsymbol{a}_\pm e^{\pm i\omega t} = 0 \Leftrightarrow (-T\omega^2 + V)\boldsymbol{a}_\pm = 0 \tag{1.11.5}$$

and we are facing an eigenvalue problem. To solve it we first need to find eigenvalues ω^2 and the determine the associated eigenvectors $\boldsymbol{a}_\pm$.

› **Example 1.2 – two coupled oscillators – using Fourier modes:**

$$m\mathbb{1}\ddot{\boldsymbol{q}} + \begin{pmatrix} k+K & -K \\ -K & k+K \end{pmatrix}\boldsymbol{q} = \boldsymbol{0} \tag{1.11.6}$$

› **Example 1.3 – two coupled oscillators – phase space method:**

To translate into phase space language we need to replace derivatives of velocieties with derivative of momenta $m\ddot{\boldsymbol{q}} = \dot{\boldsymbol{p}}$ in Eq. (1.11.6) and supplement it with $p_i = \dot{q}_i/m$. In the resulting system of equations we take the derivatives to the left

$$\dot{\boldsymbol{p}} + \begin{pmatrix} D+D_{12} & -D_{12} \\ -D_{21} & D+D_{12} \end{pmatrix}\boldsymbol{q} = \boldsymbol{0} \tag{1.11.7}$$

We end up with the homogeneous linear system

$$\begin{pmatrix} \dot{\boldsymbol{q}} \\ \dot{\boldsymbol{p}} \end{pmatrix} = \begin{pmatrix} & & 1/m & \\ & & & 1/m \\ D+D_{12} & -D_{12} & & \\ -D_{21} & D+D_{12} & & \end{pmatrix}\begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{p} \end{pmatrix} \tag{1.11.8}$$

$$\begin{pmatrix} & \begin{pmatrix} \dot{\boldsymbol{q}} \\ \\ -D_{12} \end{pmatrix} & 1/m & \\ & & & 1/m \\ D + D_{12} & & & \\ -D_{21} & D + D_{12} & & \end{pmatrix}$$

1.11.1 Linear chains

A linear chain is chain of coupled oscillators, the example of a coupled pair discussed earlier in example 1.2, page 53 is the simplest case. It would appear natural to build the more general chain with n-masses iteratively from that with $n-1$ masses. The issue with this is that one must face the presence and impact of the endpoints in every step of the construction. The *infinite* linear chain is, in fact, much simpler mathematically. We will now generalize to the case of an infinite chain of coupled oscillators. We denote the physical spacing of equilibrium positions by a. (Since this is the same mathematical setting in which condensed matter physicists discuss crystal lattices this physical distance is often generically called a lattice spacing.) The equilibrium configuration is sketched in Fig. 7.

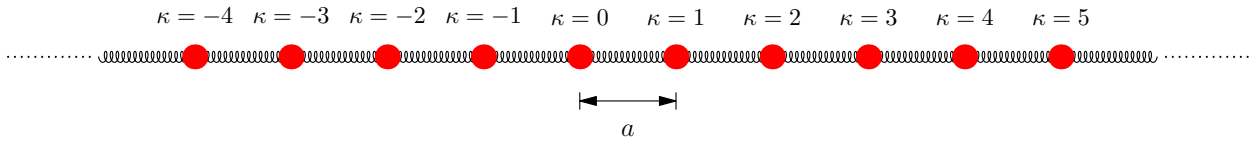


Fig. 7: *Sketch of the equilibrium configuration of an infinite linear chain of coupled harmonic oscillators, with equilibrium positions spaced a uniform lattice spacing a apart. The dots depict the masses with strings stretched between them. The integer κ labels the equilibrium locations which we will refer to as lattice sites.*

The price to pay for the infinite extension is that the potential energy stored in that system will generally become infinite, but we can retain the link with physical sanity by noting that the energy density can be kept finite. We write the energies in terms of deviations from equilibrium which we denote by $q_\kappa(t)$ where κ indexes the individual masses or equilibrium positions. Then

$$V = \frac{1}{2}\sum_{\kappa\in\mathbb{Z}} \left(md\, q_\kappa^2 + mD\,(q_\kappa - q_{\kappa+1})^2 \right) \tag{1.11.9}$$

where the constant mD represents the spring constant of the spring connecting two neighbouring masses in Fig. 7. The term proportional to md, if present, represents an additional restoring force. While the inter-mass interaction is translationally invariant along the chain (shifting all q_κ to $q_{\kappa+l}$ leaves the differences in Eq. (1.11.9) unchanged), this term breaks that symmetry.

The force on the mass at κ is then given by

$$F_\kappa = -\frac{\partial}{\partial q_\kappa} V = -mdq_\kappa - mD((q_\kappa - q_{\kappa+1}) - (q_{\kappa-1} - q_\kappa)) \tag{1.11.10}$$

(There are two terms in the sum that contain a specifc q_κ!)

Thus, its equations of motion, $m\ddot{q}_\kappa = -F_\kappa$ take the form

$$m\ddot{q}_\kappa(t) - dq_\kappa(t) - D((q_{\kappa+1}(t) - q_\kappa(t)) - (q_\kappa(t) - q_{\kappa-1}(t))) = 0 \qquad \kappa \in \mathbb{Z} \tag{1.11.11}$$

and no conditions need to be imposed at any endpoints.

We note that the equation contains a finite difference operator linking the elements along the chain (summation convention for λ!):

$$(q_{\kappa+1} - q_\kappa) - (q_\kappa - q_{\kappa-1}) = q_{\kappa+1} - 2q_\kappa + q_{\kappa-1} = (\delta_{\kappa+1,\lambda} - 2\delta_{\kappa,\lambda} + \delta_{\kappa-1,\lambda})q_\lambda =: D_{\kappa\lambda}q_\lambda \tag{1.11.12}$$

There are two useful ways to think about this operator that we will employ below:

- Clearly this behaves like a linear map. Indeed Eq. (1.11.12) displays the component form of a countably infinite dimensional band matrix of the schematic form

$$-\boldsymbol{D} := \begin{pmatrix} \ddots & \ddots & \ddots & & & & & \\ & -1 & 2 & -1 & & & & \\ & & -1 & 2 & -1 & & & \\ & & & -1 & 2 & -1 & & \\ & & & & -1 & 2 & -1 & \\ & & & & & \ddots & \ddots & \ddots \end{pmatrix} \tag{1.11.13}$$

  whose (κ, l) components are given by $D_{\kappa,\lambda}$. [The band on the diagonal corresponds to $2\delta_{\kappa,\lambda}$, the band above to $\delta_{\kappa+1,\lambda}$ and that below to $\delta_{\kappa-1,\lambda}$.] It acts on a countably infinite dimensional vector $\boldsymbol{q}$ with components q_κ. Since the matrix is symmetric, we expect it can be fully diagonalized by an orthogonal transformation (i.e. its eigenvectors can be chosen to be mutually orthogonal) and that its eigenvalues are real.

- Up to a factor $\frac{1}{\Delta^2}$, which is irrelevant for the following discussion, this indeed maps onto what is known as the *central finite difference* approximation to the second derivative along the chain

$$f''(x) \approx \frac{1}{\Delta^2}(f(x-\Delta) - 2f(x) + f(x+\Delta)) \tag{1.11.14}$$

  if we interpret the mass index as a discrete position label and the identify the step size with Δ as we have done above.

  Eq. (1.11.14) provides a good way of approximating the second derivative $(\frac{\partial}{\partial x})^2$ not least since it shares the harmonic functions as eigenfunctions:

  We observe that any infinite length vector $\boldsymbol{a}_\eta$, with components $a_{\eta,\kappa} := e^{i\eta\kappa}$, $\eta \in \mathbb{R}$, labelled by the component label $\kappa \in \mathbb{Z}$ is indeed an eigenstate of the operator $\boldsymbol{D}$ (recall there is a summation convention over λ that is employed):

$$\begin{aligned} D_{\kappa\lambda}a_{\eta,\lambda} &= (\delta_{\kappa+1\lambda} - 2\delta_{\kappa\lambda} + \delta_{\kappa-1\lambda})e^{i\eta\lambda} = (e^{i(1+\kappa)\eta} - 2e^{i\kappa\eta} + e^{i(\kappa-1)\eta}) = (e^{i\eta} - 2 + e^{-i\eta})e^{i\eta\kappa} \\ &= -2(1-\cos(\eta))a_{\eta,\kappa} = -4\sin^2(\frac{\eta}{2})a_{\eta,\kappa} \end{aligned} \tag{1.11.15}$$

  or, more compactly in matrix notation

$$\boldsymbol{D}\boldsymbol{a}_\eta = -4\sin^2(\frac{\eta}{2})\boldsymbol{a}_\eta \tag{1.11.16}$$

  Several observations are crucial to assess the consequences of this equation:

- Since the operator is real, both real and imaginary parts of $\boldsymbol{a}_\eta$ separately obey the same eigenvalue equation.
  The $\boldsymbol{a}_\eta$ represent static wave configurations imprinted on the chain. We can use the lattice spacing a to convert η to a wavenumber and an associated wavelength by defining
  $$\eta =: ka =: \frac{2\pi}{\lambda} a \tag{1.11.17}$$
  Since the components represent the locations along the chain we then see a static harmonic configuration of the form
  $$a_{\eta,\kappa} = e^{i\eta\kappa} = e^{ik\kappa a} = e^{i\frac{2\pi}{\lambda}\kappa a} \tag{1.11.18}$$
- We note that we can vary η only over finite intervals of length of 2π, say over $]-\pi, \pi[$, before the vectors repeat, since for all integer n
  $$e^{i(\eta+2\pi n)\kappa} \overset{\kappa\in\mathbb{Z}}{=} e^{i\eta\kappa} \tag{1.11.19}$$
  The interval labelling the discrete states in this and related problems is commonly called the Brillouin zone of the lattice under consideration [7, 8, 9]. This concept plays a prominent role in understanding the regular structure of crystals and the vibrational modes traveling through them. Fig. 9 exemplifies how η and $\eta' = \eta + 2\pi n$ lead to the same configuration of oscillator. The physical interpretation is clear: with a finite number of oscillators we cannot represent arbitrarily high frequencies (arbitrarily short wavelengths), wavelength shorter than $1/(2\pi)$ "fall through the gaps".
- The eigenspaces of $\boldsymbol{D}$ with eigenvalue $-4\sin^2(\frac{\eta}{2})$ at $\eta \neq 0$ are two dimensional: Both $\boldsymbol{a}_\eta$ and $\boldsymbol{a}_{-\eta}$ share the same eigenvalue and span this eigenspace: Every linear combination of the two is again an eigenvector to the same eigenvalue:
  $$\boldsymbol{D}(\alpha_\eta \boldsymbol{a}_\eta + \alpha_{-\eta}\boldsymbol{a}_{-\eta}) = -4\sin^2(\frac{\eta}{2})(\alpha_\eta \boldsymbol{a}_\eta + \alpha_{-\eta}\boldsymbol{a}_{-\eta}) \tag{1.11.20}$$
  This is the only freedom left in the choice of a complete eigensystem of $\boldsymbol{D}$.
  As we will see below, this freedom can be used to simplify the implementation of boundary conditions.

There are two complementary consequences of this discussion:

1. **The $\boldsymbol{a}_\eta$ span the space of exitations:** they obey the completeness relation
   $$\int_{-\pi}^{\pi} d\eta\; a_{\eta\kappa}(t) a_{\eta\lambda}(t)^* = \int_{-\pi}^{\pi} d\eta\; e^{i\eta(\kappa-\lambda)} = 2\pi\delta_{\kappa\lambda} \tag{1.11.21}$$
   (by explicit integration – there is no distributional finesse that comes into play here!) which states that
   $$\int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\; \boldsymbol{a}_\eta \otimes \boldsymbol{a}_\eta^\dagger = \begin{pmatrix} \ddots & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & \ddots \end{pmatrix} \tag{1.11.22}$$
   acts as the unit matrix on our infinite dimensional vector space in which our solutions $\boldsymbol{q}(t)$ take their values. This is equivalent to the statement that the states $\boldsymbol{a}_\eta$ span that vector space.

2. **The $\boldsymbol{a}_\eta$ are orthogonal for $\eta \in]-\pi,\pi[$:** That this can be done follows from an orthogonality relation of the $\boldsymbol{a}(\eta)$:

$$\boldsymbol{a}_\eta^\dagger \cdot \boldsymbol{a}_{\eta'} = \sum_{\kappa=-\infty}^{\infty} (e^{i\eta\kappa})^* e^{i\eta'\kappa} = 2\pi \sum_{n\in\mathbb{Z}} \delta(\eta - \eta' - 2\pi n) \tag{1.11.23}$$

The expression on the r.h.s. is an example of a Dirac-comb, a periodic distribution. It is this periodicity that allows the Fouier series expansion on the l.h.s.. See remark 1.5, page 71.

The completeness relation allows us to expand a general solution as

$$q_\kappa(t) = \delta_{\kappa,\lambda} q_\lambda(t) = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, a_{\eta\kappa} \underbrace{a^*_{\eta\lambda} q_\lambda(t)}_{=:Q_\eta(t)} = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, a_{\eta\kappa} Q_\eta(t) \tag{1.11.24a}$$

The orthogonality relation (1.11.23) is the complementary tool that allows us to extract the $Q_\eta(t)$ from the integral on the r.h.s. of Eq. (1.11.24a):

$$\begin{aligned} \boldsymbol{a}_\eta^\dagger \cdot \boldsymbol{q}(t) = a^*_{\eta\kappa} q_\kappa(t) = a^*_{\eta\kappa} \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, a_{\eta\kappa} Q_\eta(t) = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, a^*_{\eta\kappa} a_{\eta\kappa} Q_\eta(t) \\ = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, 2\pi \sum_{n\in\mathbb{Z}} \delta(\eta - \eta' - 2\pi n) Q_\eta(t) = Q_\eta(t) \end{aligned} \tag{1.11.24b}$$

[Note that since we restrict our superposition interval to $\eta \in]-\pi,\pi[$ we only ever encounter the $n = 0$ term of the sum over δ-distributions.]

The pair of equations (1.11.24) establishes a bijection between the $q_\kappa(t)$ and $Q_\eta(t)$ and guarantee that the map between them is an invertible change of variables. This change of variables diagonalizes the differential equation, since every $\boldsymbol{q}(t)$ can be written in the form (1.11.24a) so that

$$\begin{aligned} 0 \overset{!}{=} \Big(m\Big(\frac{d}{dt}\Big)^2 - md + mD\boldsymbol{D}\Big)\boldsymbol{q}(t) = \Big(m\Big(\frac{d}{dt}\Big)^2 - md - mD\boldsymbol{D}\Big) \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, a_{\eta\kappa} Q_\eta(t) \\ = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, \boldsymbol{a}_\eta \Big(m\Big(\frac{d}{dt}\Big)^2 - md + mD4\sin^2(\frac{\eta}{2})\Big) Q_\eta(t) \end{aligned} \tag{1.11.25}$$

Projecting this onto $\boldsymbol{a}_\eta$ (by acting with $\boldsymbol{a}_\eta^\dagger$ from the left) and using the orthogonality relation then isolates one of the linearly independent components and translates Eq. (1.11.25) into

$$0 \overset{!}{=} \Big(m(\frac{d}{dt})^2 - md + mD4\sin^2(\frac{\eta}{2})\Big) Q_\eta(t) \qquad \text{for all } \eta \in]-\pi,\pi[, \tag{1.11.26}$$

which is just the equation for a single harmonic oscillator without damping. The general solution of this single mode (fixed η) equation (1.11.26) reads

$$Q_\eta(t) = A^+_\eta e^{i\omega_\eta t} + A^-_\eta e^{-i\omega_\eta t} \tag{1.11.27}$$

where

$$\omega_\eta = \sqrt{-d + D4\sin^2(\frac{\eta}{2})} \tag{1.11.28}$$

(Note that we have explicitly chosen the positive square root solution.)

A general solution to the original equation therefore is given by

$$\boldsymbol{q}(t) = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, \boldsymbol{a}_\eta \left(A^+_\eta e^{i\omega_\eta t} + A^-_\eta e^{-i\omega_\eta t}\right) \tag{1.11.29}$$

› The relation between the frequency in the time oscillations ω_η and the spatial wave number $k = \eta/a$ is called a *dispersion relation*. The set of values of ω_η are called the *spectrum* of the underlying differential operator.

In this case the spectrum is continuous but limited to the finite interval $]-\pi, \pi[$. We will encounter more general situations with the spectrum stretched over the full real axis and more limited ones with restrictions to discretretized values. In all these cases the generic structure of the general solutions does not change, it will always be constructed by a sum or integral over the whole spectrum very similar to the expression in Eq. (1.11.27). The sums or integrals appearing in these expressions will generically be referred to as *spectral sums*, even if they are actually integrals.

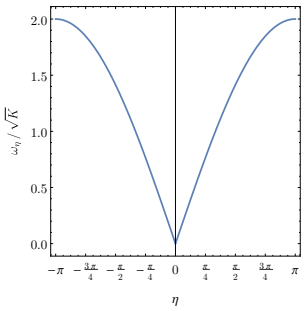


Fig. 8: *Spectrum and dispersion relation of the inifinte linear chain at $d = 0$ so that $\omega_\eta = \sqrt{D4\sin^2(\frac{\eta}{2})}$. The symmetry $\omega_\eta = \omega_{-\eta}$ imposes a twofold degeneracy at all points.*

› This general solution contains *travelling waves* present in both terms. To uncover this, we look at the components of our solution vector and recall that they represent positions along the chain.

$$q_\kappa(t) = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi} \left(A^+_\eta e^{i(\eta\kappa+\omega_\eta t)} + A^-_\eta e^{i(\eta\kappa-\omega_\eta t)}\right) \tag{1.11.30}$$

Looking at the first term, proportional to $e^{i\omega t}$, we note that it represents a left moving wave for $\eta > 0$, and a right moving wave if $\eta < 0$. At $\eta = 0$ we are looking at a synchronized collective oscillation of all members of the chain.

For the second term it is $\eta < 0$ that represents a right moving wave and $\eta > 0$ that is left moving.

We can expose them explicitly by using the $\eta \to -\eta$ symmetry of ω_η by writing

$$q_\kappa(t) = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi} \left[\frac{1}{2}\left(A^+_\eta e^{i(\eta\kappa+\omega_\eta t)} + A^+_{-\eta} e^{i(-\eta\kappa+\omega_\eta t)}\right) + \frac{1}{2}\left(A^-_\eta e^{i(\eta\kappa-\omega_\eta t)} + A^-_{-\eta} e^{i(-\eta\kappa-\omega_\eta t)}\right)\right] \tag{1.11.31}$$

› The dispersion relation (1.11.28) is symmetric under $\eta \to -\eta$, i.e. $\omega_\eta = \omega_{-\eta}$. That shows us that the time dependent solutions retain the degeneracy of the finite difference opeator $-\boldsymbol{D}$. This will allow us to impose compatible types of boundary conditions along the chain that hold for all times.

As a preview: Pinning one of the oscillators in place, say at location $\kappa = \alpha$ by imposing $q_\alpha(t) \stackrel{!}{=} 0$ *at all* t locks the relative amplidudes of the left moving wave trains with those of the associated right moving ones. It imposes $A^\pm_\eta e^{i\eta\alpha} \stackrel{!}{=} A^\pm_{-\eta} e^{-i\eta\alpha}$ for all η in the Brillouin zone. The locked element acts as a reflective boundary.

› When are the solutions real? We expect real initial conditions to lead real solutions at all times. What is the condition on the mode amplitudes

As before we will express these solutions in terms of initial conditions before we declare the homogeneous problem solved. We find

$$Q_\eta(0) = \boldsymbol{a}^\dagger_\eta \cdot \boldsymbol{q}(0) = A^+_\eta + A^-_\eta \qquad \dot{Q}_\eta(0) = \boldsymbol{a}^\dagger_\eta \cdot \dot{\boldsymbol{q}}(0) = i\omega_\eta \Big(A^+_\eta - A^-_\eta \Big) \tag{1.11.32}$$

Solving for the $A^\pm_\eta$ then leads to

$$\begin{aligned} \boldsymbol{q}(t) &= \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, \boldsymbol{a}_\eta \left[\frac{1}{2} \left(\boldsymbol{a}^\dagger_\eta \cdot \boldsymbol{q}(0) + \frac{1}{i\omega_\eta} \boldsymbol{a}^\dagger_\eta \cdot \dot{\boldsymbol{q}}(0) \right) e^{i\omega_\eta t} + \frac{1}{2} \left(\boldsymbol{a}^\dagger_\eta \cdot \boldsymbol{q}(0) - \frac{1}{i\omega_\eta} \boldsymbol{a}^\dagger_\eta \cdot \dot{\boldsymbol{q}}(0) \right) e^{-i\omega_\eta t} \right] \\ &= \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, \boldsymbol{a}_\eta \otimes \boldsymbol{a}^\dagger_\eta \left(\cos(\omega_\eta t) \boldsymbol{q}(0) + \frac{1}{\omega_\eta} \sin(\omega_\eta t) \dot{\boldsymbol{q}}(0) \right) \end{aligned} \tag{1.11.33}$$

The propagator of the single harmonic oscillator is replaced by a propagator matrix

$$\boldsymbol{P}(t-t') = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, \boldsymbol{a}_\eta \otimes \boldsymbol{a}^\dagger_\eta \frac{\sin\big(\omega_\eta (t-t')\big)}{\omega_\eta} \ . \tag{1.11.34}$$

The interpretation of the its structure is quite straightforward: The matrix structure projects onto the independent eigenmodes of the differential operator – each of these modes behave like an independent harmonic oscillator precisely the same way already encountered for that case in Eq. (1.10.19) (after we take the zero damping limit $\gamma \to 0$). Using $\boldsymbol{P}$, the general solution takes the form

$$\boldsymbol{q}(t) = \boldsymbol{P}(t-t') \dot{\boldsymbol{q}}(t') + \dot{\boldsymbol{P}}(t-t') \boldsymbol{q}(t') \tag{1.11.35}$$

in terms of initial conditions $\dot{\boldsymbol{q}}(t')$ and $\boldsymbol{q}(t')$, specified at time t'.

The Green's function that provides a solution to the inhomogeneous equation becomes

$$\boldsymbol{G}(t-t') = \int_{-\infty}^{\infty} \frac{d\tilde{\omega}}{2\pi} \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, \boldsymbol{a}_\eta \otimes \boldsymbol{a}^\dagger_\eta \frac{e^{i\tilde{\omega}(t-t')}}{-\tilde{\omega}^2 + \omega^2_\eta} = \theta(t-t') \boldsymbol{P}(t-t') \tag{1.11.36}$$

and gives access to inhomogeneous solutions

$$\boldsymbol{q}_{\boldsymbol{f}}(t) = \frac{1}{m} \int_{-\infty}^{\infty} dt'\ \boldsymbol{G}(t-t') \boldsymbol{f}(t') \tag{1.11.37}$$

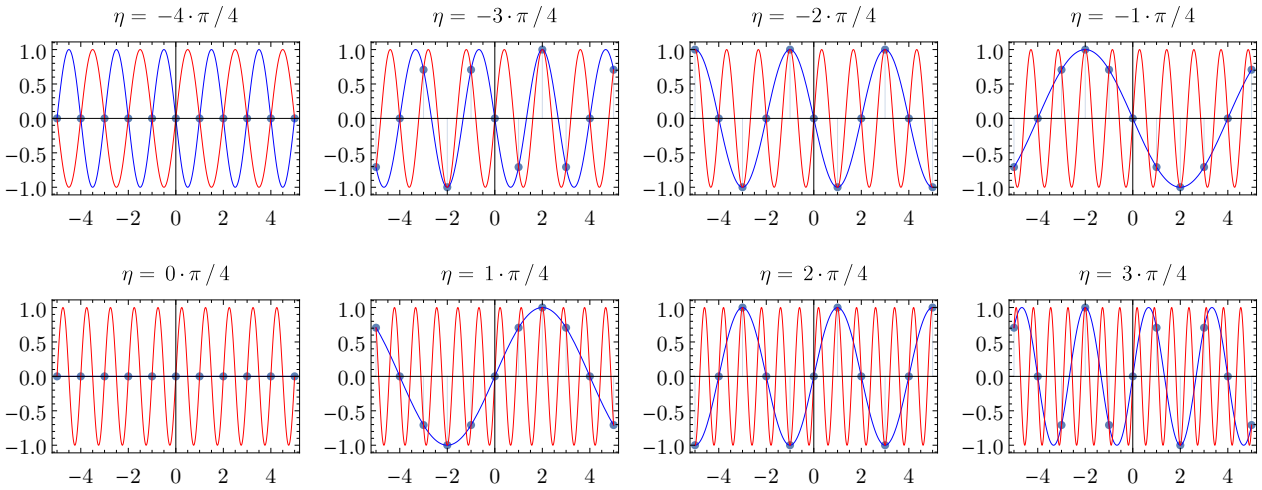


Fig. 9: $\sin(\eta\kappa)$, *the imaginary part of* $e^{i\eta\kappa}$ *as a function of* $\kappa \in \mathbb{Z}$ *as represented by the oscillators on a linear chain (dots). The sequence of plots scans* $\eta \in [-\pi, \pi[$ *in steps of* $\pi/4$. *Overlaid are* $\sin(\eta x)$ *(blue) and* $\sin((\eta + 2\pi)x)$ *(red). This illustrates the general case: The positions of the oscillators are identical for* η *and* $\eta + 2\pi$. *The physical interpretation is clear: Wavelengths shorter than* $1/\eta = 1/(2\pi)$ *cannot be represented by the discrete set of oscillators. The discrete spacing provides a frequency cutoff.*

The Green's functions and propagators are real, and thus turn real initial consitions and forces into real solutions!

› **Example 1.4 – forcing a single element on the chain:**

We apply a harmonic force to the chain by that acts only at a single location $\kappa = \alpha$, i.e. we choose $\boldsymbol{f}$ of Eq. (1.11.37) to have a single component $f_\kappa(t) = \delta_{\kappa,\alpha} m f_0 \sin(\Omega t)$ (f_0 has units of [force/mass]!). The main difference to the single harmonic oscillator is that the coupled linear chain has (infinitely) many eigenmodes we need to couple to.

The most efficient way to go about this is to use the Fourier representation of $\boldsymbol{G}$, Eq. (1.11.36). We

work in component notation to expose the individual harmonics:

$$\begin{aligned}
q_{\boldsymbol{f},\kappa}(t) &= \frac{1}{m}\int_{-\infty}^{\infty} dt'\; G_{\kappa\lambda}(t-t')f_\lambda(t') \\
&= \frac{1}{m}\int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty}\frac{d\tilde{\omega}}{2\pi}\int_{-\pi}^{\pi}\frac{d\eta}{2\pi}\; a_{\eta\kappa}a^*_{\eta\lambda}\frac{e^{i\tilde{\omega}(t-t')}}{-\tilde{\omega}^2+\omega_\eta^2}\delta_{\lambda,\alpha}mf_0\sin(\Omega t) \\
&= \frac{1}{m}\int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty}\frac{d\tilde{\omega}}{2\pi}\int_{-\pi}^{\pi}\frac{d\eta}{2\pi}\; e^{i\eta(\kappa-\alpha)}\frac{e^{i\tilde{\omega}(t-t')}}{-\tilde{\omega}^2+\omega_\eta^2}\delta_{\lambda,\alpha}mf_0\frac{1}{2i}\left(e^{i\Omega t'}-e^{-i\Omega t'}\right) \\
&= f_0\int_{-\infty}^{\infty} d\tilde{\omega} \int_{-\pi}^{\pi}\frac{d\eta}{2\pi}\; e^{i\eta(\kappa-\alpha)}\frac{e^{i\tilde{\omega}t}}{-\tilde{\omega}^2+\omega_\eta^2}\frac{1}{2i}\left(\delta(\tilde{\omega}-\Omega)-\delta(\tilde{\omega}+\Omega)\right) \\
&= f_0\int_{-\pi}^{\pi}\frac{d\eta}{2\pi}\; e^{i\eta(\kappa-\alpha)}\frac{1}{-\Omega^2+\omega_\eta^2}\frac{1}{2i}\left(e^{i\Omega t}-e^{-i\Omega t}\right) \qquad (1.11.38)
\end{aligned}$$

Using the $\eta \mapsto -\eta$ symmetry of the denominator we can rewrite this as

$$\begin{aligned}
(1.11.38) &= f_0\int_{-\pi}^{\pi}\frac{d\eta}{2\pi}\; \frac{1}{-\Omega^2+\omega_\eta^2}\frac{1}{2i}\left(e^{i(\eta(\kappa-\alpha)+\tilde{\Omega}t)}-e^{-i(\eta(\kappa-\alpha)+\tilde{\Omega}t)}\right) \\
&= f_0\int_{-\pi}^{\pi}\frac{d\eta}{2\pi}\; \frac{1}{-\Omega^2+\omega_\eta^2}\sin(\eta(\kappa-\alpha)+\tilde{\Omega}t) \qquad (1.11.39)
\end{aligned}$$

and you might be tempted to interpret this as a superposition of travelling waves, and a travelling wave altogether?

However, if we proceed differently, we obtain

$$\begin{aligned}
(1.11.38) &= f_0\int_{-\pi}^{\pi}\frac{d\eta}{2\pi}\; e^{i\eta(\kappa-\alpha)}\frac{1}{-\Omega^2+\omega_\eta^2}\sin(\Omega t) \\
&= f_0\int_{-\pi}^{\pi}\frac{d\eta}{2\pi}\; \cos(\eta(\kappa-\alpha))\frac{1}{-\Omega^2+\omega_\eta^2}\sin(\Omega t) \qquad (1.11.40)
\end{aligned}$$

This looks like a superposition of standing waves! How do entice this to travel?

If I employ my intuition I would expect energy transport to happen away from the force acting at α,

something like

$$(1.11.38) = f_0 \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\ \cos(\eta(\kappa-\alpha))\frac{1}{-\Omega^2+\omega_\eta^2}\sin(\Omega t)$$
$$\stackrel{?}{=} f_0 \int_{0}^{\pi} \frac{d\eta}{2\pi}\ \frac{1}{-\Omega^2+\omega_\eta^2}\left(\theta(\alpha-\kappa)\sin(\eta(\kappa-\alpha)+\Omega t)+\theta(\kappa-\alpha)\sin(\eta(\kappa-\alpha)+\Omega t)\right) \tag{1.11.41}$$

Remark 1.13 – mode expansions of real mode vectors:

We can always apply our original mode expansions to both the homogeneous initial conditions (both locations and velocities) and the force alike, but we need to ensure they come out to be real:

$$\boldsymbol{q}(t') = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\ \boldsymbol{a}_\eta Q_\eta(t') \stackrel{!}{=} \boldsymbol{q}^*(t') = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\ \boldsymbol{a}_{-\eta} Q_\eta^*(t') = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\ \boldsymbol{a}_\eta Q_{-\eta}^*(t') \tag{1.11.42}$$

where we have used that $\boldsymbol{a}_\eta^* = \boldsymbol{a}_{-\eta}$ and substituted $\eta \to -\eta$ to arrive at the final expression. Projecting onto $\boldsymbol{a}_\eta$ (by acting with $\boldsymbol{a}_\eta^\dagger$ from the left) we obtain the condition

$$Q_{-\eta}(t') \stackrel{!}{=} Q_\eta^*(t') \tag{1.11.43}$$

If condition (1.11.43) holds we can simply take the real part without losing information:

$$\begin{aligned} q_\kappa(t') &= \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\ a_{\eta\kappa} Q_\eta(t') \\ &= \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\left(\frac{1}{2}(a_{\eta\kappa}+a_{-\eta\kappa})\frac{Q_\eta(t')+Q_\eta^*(t')}{2} - \frac{1}{2i}(a_{\eta\kappa}-a_{-\eta\kappa})\frac{Q_\eta(t')-Q_\eta^*(t')}{2i}\right) \\ &= \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\left(\cos(\eta\kappa)\mathsf{Re}(Q_\eta(t')) + \sin(\eta\kappa)(-\mathsf{Im}(Q_\eta(t')))\right) \\ &= \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}|Q_\eta(t')|\sin(\eta\kappa+\phi) \end{aligned} \tag{1.11.44}$$

where

$$\sin(\phi) := \frac{\mathsf{Re}(Q_\eta(t'))}{|Q_\eta(t')|} \qquad \text{and consistently} \qquad \cos(\phi) := -\frac{\mathsf{Im}(Q_\eta(t'))}{|Q_\eta(t')|} \tag{1.11.45}$$

The same condition applies to the expansion coefficients in the mode expansions of initial velocities and real forces.

The infinite homogeneous chain of oscillators would, at first sight, appear to be a very special case of a general system of oscillators. In fact it provides a beautiful starting point to analyse other systems. For example, we can easily imagine that in any physical realization of an infinite chain we pinch two of the oscillating masses, leaving precisely n masses between the ones we lock at the $q = 0$ position. This clearly decouples the infinite chain into three independent subsystems. The isolated subsystem between the pinches is a linear chain with n-oscillators. The systems to either side are coupled oscillators with one fixed endpoint that we will learn to interpret as a reflecting wall.

There is no direct provision for pinching fingers in our calculation setup, so how do we implement that *mathematically*?

This would at first appear to be more than we can easily do with only a restriction of the intial conditions: after all, we require the two oscillators at the pinching locations to remain locked in position *for all times*!

The answer to this question will be that this is only an apparent difficulty and that we can achieve that goal by restricting the spectrum of allowed oscillations, we need to place restrictions on the $Q_\eta(t')$ at initial time!

Imposing periodicity after n steps $q_{\kappa+2\pi n} \stackrel{!}{=} q_\kappa$ is possible in the same manner. This will be discussed in more detail below.

$$P_{\kappa\lambda}(t-t') = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, e^{i\eta(\kappa-\lambda)} \frac{\sin\big(\omega_\eta(t-t')\big)}{\omega_\eta} \qquad \dot{P}_{\kappa\lambda}(t-t') = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, e^{i\eta(\kappa-\lambda)} \cos\big(\omega_\eta(t-t')\big) \quad (1.11.46)$$

If the other modes are not allowed to propagate into $\kappa = 0$ we need $P_{0\lambda} = 0$ and $\dot{P}_{0\lambda} = 0$ for all times! A whole column of the associated propagator must vanish. At the same time one needs to retain the conditions $P(0) = 0$ and $\dot{P}(0) = 1$.

› **Example 1.5 – the linear chain with a reflective wall:**

We now want to pin *one* of the oscillators, say at location α, at its equilibrium position $q_\alpha(t) = 0$ *for all times*.

Looking at the eigensolutions at fixed η, $A^+_\eta e^{i(\eta\kappa+\omega_\eta t)} + A^-_\eta e^{i(\eta\kappa-\omega_\eta t)}$ we see that none of them behave that way. Are we out of luck? Surely not since we can certainly physically carry this out in an experiment.

What allows us to do this *mathematically* is the fact that the solutions at η and $-\eta$ are degenerate and correspond to the same ω_η. As we have noted in Eq. (1.11.31), this puts left and right moving waves into the same eigenspace so that we can form linear combinations of the form

$$A^+_\eta e^{i(\eta\kappa+\omega_\eta t)} + A^+_{-\eta} e^{i(-\eta\kappa+\omega_\eta t)} = \big(A^+_\eta e^{i\eta\kappa} + A^+_{-\eta} e^{-i\eta\kappa}\big)\, e^{i\omega_\eta t} \quad (1.11.47)$$

which are eigenstates of $\boldsymbol{D}$, irrespective of the coefficients. Since this linear combination shares a common time dependence it can be pinned to zero for all times at $\kappa = \alpha$, simply by setting the amplitude at $\kappa = \alpha$ to zero:

$$0 \stackrel{!}{=} A^+_\eta e^{i\eta\alpha} + A^+_{-\eta} e^{-i\eta\alpha}\ . \quad (1.11.48)$$

This procedure selects a state proportional to $\boldsymbol{a}_\eta - \boldsymbol{a}_{-\eta} e^{i2\eta\alpha}$. The associated propagating mode is

proportional to

$$(\boldsymbol{a}_\eta - \boldsymbol{a}_{-\eta} e^{i2\eta\alpha}) e^{i\omega_\eta t} \tag{1.11.49}$$

It is a standing wave that emerges as a superposition of a left and a right moving wave that destructively interfere at $\kappa = \alpha$ to form a node at all times. Enforcing this node at all times removes half of the degrees of freedom by linking the amplitudes of left and right moving solutions.

At fixed η, the result is a standing wave with one of the nodes fixed at $\kappa = \alpha$ whose amplitudes oscillate in place with a wavelength according to $\lambda = \frac{2\pi}{\eta}$ as illustrated in Fig. 10. This implies that:

- The standing waves are reflection symmetric around the pinned location at $\kappa = \alpha$.
- All node locations other than that at $\kappa = \alpha$ are η dependent. This is illustrated in Fig. 10
- Longitudinal movement arises only through superposition of modes with diffent η values.

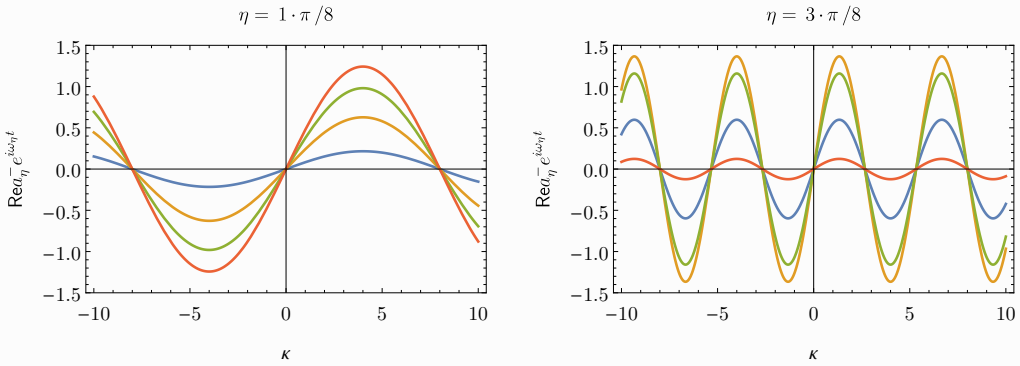


Fig. 10: *Wave solutions pinned at $\kappa = 0$ shown for different values of t. The solutions are standing waves that exhibit a reflection symmetry around the pinning location. The node locations other than that at the reflecting wall are η dependent.*

Solving (1.11.48) and inserting the outcome into the general mode expansion for a homogeneous solution (1.11.29) solves the homogeneous problem completely.

If one is interested in the general initial value problem and in inhomogeneous solutions as well, one needs to work a little more. One needs to upgrade the discussion to a complete change of basis that allows us to provide an adapted analogue for the expressions of the propagator $\boldsymbol{P}(t - t')$ and with it, for the Green's function $\boldsymbol{G}(t - t')$.

A convenient choice for the states selected by Eq. (1.11.50) is

$$\boldsymbol{a}^-_\eta := \frac{1}{\sqrt{2}} \left(\boldsymbol{a}_\eta e^{-i\eta\alpha} - \boldsymbol{a}_{-\eta} e^{i\eta\alpha} \right) \tag{1.11.50}$$

whose components

$$a^-_{\eta,\kappa} = \frac{1}{\sqrt{2}}\left(e^{i\eta(\kappa-\alpha)} - e^{-i\eta(\kappa-\alpha)}\right) \tag{1.11.51}$$

indeed vanish at $\kappa = \alpha$ as advertised.

Any two such states are orgthogonal and δ normalized, just as the $\boldsymbol{a}_\eta$ themselves:

$$\frac{1}{2}\left(\boldsymbol{a}_\eta e^{i\eta\alpha} - \boldsymbol{a}_{-\eta}e^{-i\eta\alpha}\right)^\dagger\left(\boldsymbol{a}_\eta e^{i\eta\alpha} - \boldsymbol{a}_{-\eta}e^{-i\eta\alpha}\right) = \frac{1}{2}\left(\boldsymbol{a}^\dagger_\eta\boldsymbol{a}_\eta + \boldsymbol{a}^\dagger_{-\eta}\boldsymbol{a}_{-\eta}\right) = 2\pi\sum_{n\in\mathbb{Z}}\delta(\eta-\eta'-2\pi n) \tag{1.11.52}$$

To span the two dimensional solution space of the left and right moving waves we need an orthogonal state, a state $\boldsymbol{a}^+_\eta$ such that $(\boldsymbol{a}^-_\eta)^\dagger\cdot\boldsymbol{a}^+_\eta = 0$. An obvious choice is

$$\boldsymbol{a}^+_\eta = \frac{1}{\sqrt{2}}\left(\boldsymbol{a}_\eta e^{-i\eta\alpha} + \boldsymbol{a}_{-\eta}e^{i\eta\alpha}\right) \tag{1.11.53}$$

These are always finite at $\kappa = \alpha$.

The inverse transformation is

$$\boldsymbol{a}_\eta = \frac{1}{\sqrt{2}}\left(\boldsymbol{a}^-_\eta e^{i\eta\alpha} + \boldsymbol{a}^+_\eta e^{-i\eta\alpha}\right) \qquad \boldsymbol{a}_{-\eta} = \frac{1}{\sqrt{2}}\left(\boldsymbol{a}^-_\eta e^{i\eta\alpha} - \boldsymbol{a}^+_\eta e^{-i\eta\alpha}\right) \tag{1.11.54}$$

We get both $\boldsymbol{a}_\eta$ and $\boldsymbol{a}_{-\eta}$ from the $\boldsymbol{a}^\pm_\eta$ with positive η. Thus, if we want to use these as basis states, we must restrict the spectral sum (the integral over η) to positive η values, the interval $]0,\pi[$. The completeness splits:

$$\int_0^\pi \frac{d\eta}{2\pi}[\boldsymbol{a}^-_\eta\otimes(\boldsymbol{a}^-_\eta)^\dagger]_{\kappa\lambda} = \frac{1}{2}\Big(\delta_{\kappa,\lambda} - \delta_{\kappa-\alpha,-(\lambda-\alpha)}\Big) \tag{1.11.55}$$

and

$$\int_0^\pi \frac{d\eta}{2\pi}[\boldsymbol{a}^+_\eta\otimes(\boldsymbol{a}^+_\eta)^\dagger]_{\kappa\lambda} = \frac{1}{2}\Big(\delta_{\kappa,\lambda} + \delta_{\kappa+\lambda,2\alpha}\Big) = \delta_{\kappa,\lambda} - \frac{1}{2}\Big(\delta_{\kappa,\lambda} - \delta_{\kappa+\lambda,2\alpha}\Big) \tag{1.11.56}$$

become mutually orthogonal projection operators, so that

$$\int_{-\pi}^\pi \frac{d\eta}{2\pi}\; a_{\eta\kappa}a^*_{\eta\lambda} = \int_0^\pi \frac{d\eta}{2\pi}\;\left(a^+_{\eta\kappa}(a^+_{\eta\lambda})^* + a^-_{\eta\kappa}(a^-_{\eta\lambda})^*\right) = \delta_{\kappa\lambda} \tag{1.11.57}$$

The full solution of the general infinite chain can be rewritten as

$$\begin{aligned}\boldsymbol{q}(t) &= \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, \boldsymbol{a}_\eta \left(A_\eta^+ e^{i\omega_\eta t} + A_\eta^- e^{-i\omega_\eta t}\right) \\ &= \int_{0}^{\pi} \frac{d\eta}{2\pi}\, \left[\boldsymbol{a}_\eta \left(A_\eta^+ e^{i\omega_\eta t} + A_\eta^- e^{-i\omega_\eta t}\right) + \boldsymbol{a}_{-\eta} \left(A_{-\eta}^+ e^{-i\omega_\eta t} + A_{-\eta}^- e^{i\omega_\eta t}\right)\right] \\ &= \int_{0}^{\pi} \frac{d\eta}{2\pi}\, \left[\boldsymbol{a}_\eta^- \left(\tilde{A}_\eta^+ e^{i\omega_\eta t} + \tilde{A}_\eta^- e^{-i\omega_\eta t}\right) + \boldsymbol{a}_\eta^+ \left(\tilde{B}_\eta^+ e^{i\omega_\eta t} + \tilde{B}_\eta^- e^{-i\omega_\eta t}\right)\right] \end{aligned} \tag{1.11.58}$$

In this form it becomes obvious that the desired pinned solution is the special case with $\tilde{B}_\eta^\pm = 0$.

Both propagator and Green's function can be expressed in the new basis

$$\boldsymbol{P}(t-t') = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, \boldsymbol{a}_\eta \otimes \boldsymbol{a}_\eta^\dagger \frac{\sin\big(\omega_\eta(t-t')\big)}{\omega_\eta} = \int_{0}^{\pi} \frac{d\eta}{2\pi}\, \left(\boldsymbol{a}_\eta^- \otimes (\boldsymbol{a}_\eta^-)^\dagger + \boldsymbol{a}_\eta^+ \otimes (\boldsymbol{a}_\eta^+)^\dagger\right) \frac{\sin\big(\omega_\eta(t-t')\big)}{\omega_\eta}\,. \tag{1.11.59}$$

which immediately allows us to conclude that an initial condition that has only $\boldsymbol{a}_\eta^-$ modes in both initial positions $\boldsymbol{q}(t')$ and initial velocities $\dot{\boldsymbol{q}}(t')$ will preserve the pinned position of the mass at location α. The same applies to the reaction to external forces.

- But are the pieces real?
- How do we split the system into two halves?

$$\begin{aligned}\boldsymbol{a}_\eta \otimes \boldsymbol{a}_\eta^\dagger &= \frac{1}{2}\left(\boldsymbol{a}_\eta^- e^{i\eta\alpha} - \boldsymbol{a}_\eta^+ e^{-i\eta\alpha}\right)\left(\boldsymbol{a}_\eta^- e^{i\eta\alpha} - \boldsymbol{a}_\eta^+ e^{-i\eta\alpha}\right)^\dagger \\ &= \frac{1}{2}\left(\boldsymbol{a}_\eta^- \otimes (\boldsymbol{a}_\eta^-)^\dagger + \boldsymbol{a}_\eta^- \otimes (\boldsymbol{a}_\eta^+)^\dagger e^{i2\eta\alpha} + \boldsymbol{a}_\eta^+ \otimes (\boldsymbol{a}_\eta^-)^\dagger e^{-i2\eta\alpha} + \boldsymbol{a}_\eta^+ \otimes (\boldsymbol{a}_\eta^+)^\dagger\right) \end{aligned} \tag{1.11.60}$$

The mixed terms cancel if we symmetrize in $\eta \to -\eta$.

Conversely

$$\begin{aligned}[\boldsymbol{a}_\eta^- \otimes (\boldsymbol{a}_\eta^-)^\dagger]_{\kappa\lambda} &= \frac{1}{2}\left(e^{i\eta(\kappa-\alpha)} - e^{-i\eta(\kappa-\alpha)}\right)\left(e^{i\eta(\lambda-\alpha)} - e^{-i\eta(\lambda-\alpha)}\right)^* \\ &= \frac{1}{2}\left(e^{i\eta(\kappa-\lambda)} - e^{i\eta(\kappa+\lambda-2\alpha)} - e^{-i\eta(\kappa+\lambda-2\alpha)} + e^{-i\eta(\kappa-\lambda)}\right) \end{aligned} \tag{1.11.61}$$

and

$$\begin{aligned}[\boldsymbol{a}_\eta^+ \otimes (\boldsymbol{a}_\eta^+)^\dagger]_{\kappa\lambda} &= \frac{1}{2}\left(e^{i\eta(\kappa-\alpha)} + e^{-i\eta(\kappa-\alpha)}\right)\left(e^{i\eta(\lambda-\alpha)} + e^{-i\eta(\lambda-\alpha)}\right)^* \\ &= \frac{1}{2}\left(e^{i\eta(\kappa-\lambda)} + e^{i\eta(\kappa+\lambda-2\alpha)} + e^{-i\eta(\kappa+\lambda-2\alpha)} + e^{-i\eta(\kappa-\lambda)}\right) \end{aligned} \tag{1.11.62}$$

are both real.

We observe that

$$\int_0^\pi \frac{d\eta}{2\pi}[\boldsymbol{a}_\eta^- \otimes (\boldsymbol{a}_\eta^-)^\dagger]_{\kappa\lambda} = \frac{1}{2}\Big(\delta_{\kappa,\lambda} - \delta_{\kappa-\alpha,-(\lambda-\alpha)}\Big) \tag{1.11.63}$$

$$\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix} \tag{1.11.64}$$

This structure

- nixes everything a α: the αth row and column are both thoroughly zero!
- But it does not decouple: it *reflects* at α (the -1 contributions)!

Still, it is a projection operator? (The sum is over all $\rho \in \mathbb{Z}$)

$$\begin{aligned}
&\frac{1}{2}\Big(\delta_{\kappa,\rho} - \delta_{\kappa+\rho,2\alpha}\Big)\frac{1}{2}\Big(\delta_{\rho,\lambda} - \delta_{\rho+\lambda,2\alpha}\Big) = \frac{1}{4}\Big(\delta_{\kappa,\lambda} - \delta_{\kappa+\lambda,2\alpha} - \delta_{\kappa+\lambda,2\alpha} + \delta_{-\kappa+2\alpha,\rho}\delta_{\rho,2\alpha-\lambda}\Big) \\
=&\frac{1}{4}\Big(\delta_{\kappa,\lambda} - \delta_{\kappa+\lambda,2\alpha} - \delta_{\kappa+\lambda,2\alpha} + \delta_{-\kappa+2\alpha,2\alpha-\lambda}\Big) = \frac{1}{2}\Big(\delta_{\kappa,\lambda} - \delta_{\kappa+\lambda,2\alpha}\Big)
\end{aligned} \tag{1.11.65}$$

This works but we see that we combine terms from both sides of α to get this.

The same applies to its complement

$$\int_0^\pi \frac{d\eta}{2\pi}[\boldsymbol{a}_\eta^+ \otimes (\boldsymbol{a}_\eta^+)^\dagger]_{\kappa\lambda} = \frac{1}{2}\Big(\delta_{\kappa,\lambda} + \delta_{\kappa+\lambda,2\alpha}\Big) = \delta_{\kappa,\lambda} - \frac{1}{2}\Big(\delta_{\kappa,\lambda} - \delta_{\kappa+\lambda,2\alpha}\Big) \tag{1.11.66}$$

Can we first symmetrize and antisymmetrize around α?

Example 1.6 – the linear chain with n-oscillators, locked at two positions:

This is can easily be realized by subjecting the infinite linear chain to the constraint that the masses at positions α and $\beta = a + n + 1$ are held fixed at zero. The general setting can accommodate this, since both the amplitudes and η are yet unconstrained.

To see whether the infinite chain admits solutions of this type we consider its eigenmode expansions at

initial time t' (and take into account that we are looking for a real mode expansion)

$$q_\kappa(t') = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, a_{\eta\kappa} Q_\eta(t') = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi} \left(\cos(\eta\kappa)\mathsf{Re}(Q_\eta(t')) + \sin(\eta\kappa)(-\mathsf{Im}(Q_\eta(t')))\right) \ , \tag{1.11.67}$$

which holds of $Q_{-\eta}(t') = Q^*_\eta(t')$ as discussed in remark 1.13 on page 62.

The same remark demonstrates that we can use the Q_η to shift the result to arbitraty values of α by tayloring the phase of Q_η accordingly. We use this to simplify our task and set $\alpha = 0$ and, hence $\beta = n + 1$ – this will fix the phase of Q_η below.

Clearly we can enforce $q_0(t') \stackrel{!}{=} q_{n+1}(t') \stackrel{!}{=} 0$ by setting the integrand to zero at those locations. This yields the conditions

$$\begin{aligned} 0 &= a_{\eta 0} Q_\eta(t') = \mathsf{Re}Q_\eta(t')\cos(\eta 0) - \mathsf{Im}Q_\eta(t')\sin(\eta 0) = \mathsf{Re}Q_\eta(t')\alpha \\ 0 &= a_{\eta(n+1)} Q_\eta(t') = \mathsf{Re}Q_\eta(t')\cos(\eta(n+1)) - \mathsf{Im}Q_\eta(t')\sin(\eta(n+1)) \\ &= -\mathsf{Im}Q_\eta(t')\sin(\eta(n+1)) \Leftrightarrow \eta(n+1) = \pi r, r \in \mathbb{Z} \end{aligned} \tag{1.11.68}$$

The eigenstates selected by this criterion at fixed κ are proportional and thus degenerate for $\pm r$:

$$\sin(\eta_r\kappa) = \sin(\frac{\pi}{n+1} r\kappa) = -\sin(\frac{\pi}{n+1}(-r)\kappa) \tag{1.11.69}$$

If we assume these to constitute the full set of allowed contributions we get that

$$Q_\eta(t') = i\mathsf{Im}Q_\eta(t') \sum_{r=1}^{n} \delta(\eta - \eta_r) \qquad \text{where} \qquad \eta_r := \frac{\pi}{n+1} r \tag{1.11.70}$$

so that

$$q_\kappa(t') = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi} \sin(\eta\kappa)(-\mathsf{Im}(Q_\eta(t'))) = \sum_{r=1}^{n} \frac{-\mathsf{Im}(Q_{\eta_r}(t'))}{2\pi} \sin(\eta_r\kappa) \tag{1.11.71}$$

To understand if the n states

(1.11.72)

span the *full* space of solutions we need to see if they form a complete se

As it turns out the orthogonality and completeness relations are structurally identical. They read

$$\sum_{r=1}^{n} \sin(\frac{\pi r}{n+1}\kappa)\sin(\frac{\pi r}{n+1}\lambda) = \frac{n+1}{2}\delta_{\kappa\lambda} \text{ for all } \kappa, \lambda \in (1:n) \tag{1.11.73}$$

for the completeness relation, and

$$\sum_{\kappa=1}^{n} \sin(\frac{\pi r}{n+1}\kappa)\sin(\frac{\pi s}{n+1}\kappa) = \frac{n+1}{2}\delta_{rs} \text{ for all } r,s \in (1:n) \tag{1.11.74}$$

for orthogonality. The proof of one also proves the other. (See aside 1.14 on page 70.) This procedure in fact physically decouples the n oscillators from the rest. Indeed since the special solutions are eigensolutions, i.e.

$$\begin{pmatrix}
\ddots & \ddots & \ddots & & & & & & & & & \\
 & -1 & 2 & -1 & & & & & & & & \\
 & & -1 & 2 & -1 & & & & & & & \\
 & & & -1 & 2 & -1 & & & & & & \\
 & & & & -1 & 2 & -1 & & & & & \\
 & & & & & \ddots & \ddots & \ddots & & & & \\
 & & & & & & -1 & 2 & -1 & & & \\
 & & & & & & & -1 & 2 & -1 & & \\
 & & & & & & & & -1 & 2 & -1 & \\
 & & & & & & & & & \ddots & \ddots & \ddots
\end{pmatrix}
\begin{pmatrix} \vdots \\ q_{-1}(\eta_r) \\ 0 \\ q_1(\eta_r) \\ q_2(\eta_r) \\ \vdots \\ q_{n-1}(\eta_r) \\ q_n(\eta_r) \\ 0 \\ q_{n+2}(\eta_r) \\ \vdots \end{pmatrix}
= 4\sin^2(\frac{\eta_r}{2})
\begin{pmatrix} \vdots \\ q_{-1}(\eta_r) \\ 0 \\ q_1(\eta_r) \\ q_2(\eta_r) \\ \vdots \\ q_{n-1}(\eta_r) \\ q_n(\eta_r) \\ 0 \\ q_{n+2}(\eta_r) \\ \vdots \end{pmatrix} \tag{1.11.75}$$

[The zeroes on the right are an algebraic consequence of $q_{\kappa+1}(\eta_r) + q_{\kappa-1}(\eta_r)$ at $\kappa = a, b$ imposed by our specific solutions!] we may as well simplify the matrix by deleting ath row and column pair and do the same at b to write a simplified matrix that represents the same linear map as $\boldsymbol{D}$ on the restricted space imposed by the conditions (1.11.68):

$$\begin{pmatrix}
\ddots & \ddots & \ddots & & & & & & & & & \\
 & -1 & 2 & 0 & & & & & & & & \\
 & & 0 & 0 & 0 & & & & & & & \\
 & & & 0 & 2 & -1 & & & & & & \\
 & & & & -1 & 2 & -1 & & & & & \\
 & & & & & \ddots & \ddots & \ddots & & & & \\
 & & & & & & -1 & 2 & -1 & & & \\
 & & & & & & & -1 & 2 & 0 & & \\
 & & & & & & & & 0 & 0 & 0 & \\
 & & & & & & & & & 0 & 2 & -1 \\
 & & & & & & & & & & \ddots & \ddots & \ddots
\end{pmatrix}
\begin{pmatrix} \vdots \\ q_{-1}(\eta_r) \\ 0 \\ q_1(\eta_r) \\ q_2(\eta_r) \\ \vdots \\ q_{n-1}(\eta_r) \\ q_n(\eta_r) \\ 0 \\ q_{n+2}(\eta_r) \\ \vdots \end{pmatrix}
= 4\sin^2(\frac{\eta_r}{2})
\begin{pmatrix} \vdots \\ q_{-1}(\eta_r) \\ 0 \\ q_1(\eta_r) \\ q_2(\eta_r) \\ \vdots \\ q_{n-1}(\eta_r) \\ q_n(\eta_r) \\ 0 \\ q_{n+2}(\eta_r) \\ \vdots \end{pmatrix} \tag{1.11.76}$$

The subspace of vectors $(q_1(\eta_r), \ldots, q_n(\eta_r))^t$ fully decouples and reproduces the problem of n identical coupled oscillators:

$$\begin{pmatrix}
2 & -1 & & & \\
-1 & 2 & -1 & & \\
 & \ddots & \ddots & \ddots & \\
 & & -1 & 2 & -1 \\
 & & & -1 & 2
\end{pmatrix}
\begin{pmatrix} q_1(\eta_r) \\ q_2(\eta_r) \\ \vdots \\ q_{n-1}(\eta_r) \\ q_n(\eta_r) \end{pmatrix}
= 4\sin^2(\frac{\eta_r}{2})
\begin{pmatrix} q_1(\eta_r) \\ q_2(\eta_r) \\ \vdots \\ q_{n-1}(\eta_r) \\ q_n(\eta_r) \end{pmatrix} \tag{1.11.77}$$

Since now we are working with symmetric linear maps on a fininte dimensional vector space we can normalize our eigenvectors:

$$\boldsymbol{q}^t(\eta_r)\cdot\boldsymbol{q}(\eta_s)=\sum_{\kappa=1}^{n}\sin\qquad\forall\eta\neq\eta'\in]0,2\pi[\tag{1.11.78}$$

https://math.stackexchange.com/questions/1880622/orthogonality-of-discrete-sine-functior

Remark 1.14 – proving completeness and orthogonality of $\sin(\frac{\pi}{n+1}r\kappa)$:

This aside provides the proofs for the orthogonality and completeness relations used to solve the finite chain with fixed boundary conditions, Eqns. (1.11.73) and (1.11.74), the completeness relation

$$\sum_{r=1}^{n}\sin(\frac{\pi r}{n+1}\kappa)\sin(\frac{\pi r}{n+1}\lambda)=\frac{n+1}{2}\delta_{\kappa\lambda}\text{ for all }\kappa,\lambda\in(1:n) \tag{1.11.79}$$

accompanied by the orthogonality statement

$$\sum_{\kappa=1}^{n}\sin(\frac{\pi r}{n+1}\kappa)\sin(\frac{\pi s}{n+1}\kappa)=\frac{n+1}{2}\delta_{rs}\text{ for all }r,s\in(1:n) \tag{1.11.80}$$

It is *not* a surprise that the states are mutually orthogonal – they are eigenstates of a symmetric linear map to distinct eigenvalues after all. What is not so obvious are the normalization factors that appear on on the right. They need to be derived.

I distinctly remember to be flummoxed when I first encountered the orthogonality relations in Kuypers' mechanics textbook [10] as a student. Sums are more complicated than integals and feature even less in undergradute curricula. The present need to verify these expressions is a good opportunity to see an example of the art. I have learned the trick employed below from Julius Wess, [11] Sec. 22. Unfortunately, both texts do not appear to have an English language edition.

We start from

$$\begin{aligned}&\sum_{\kappa=1}^{n}\sin(\frac{\pi r}{n+1}\kappa)\sin(\frac{\pi s}{n+1}\kappa)\\&=\sum_{\kappa=1}^{n}\frac{1}{(2i)^2}\left(e^{i\frac{\pi}{n+1}(r+s)\kappa}-e^{i\frac{\pi}{n+1}(r-s)\kappa}-e^{-i\frac{\pi}{n+1}(r-s)\kappa}+e^{-i\frac{\pi}{n+1}(r+s)\kappa}\right)\end{aligned} \tag{1.11.81}$$

and need to evaluate the sums.

I have decomposed the product of two sin functions into four separate exponentials, since in this form, we can use an expression for the partial sums of the geometric series to evaluate the sums involved:

$$\sum_{\kappa=0}^{n-1}x^\kappa=\frac{1-x^n}{1-x} \tag{1.11.82}$$

As a function of x this is even smooth at $x = 1$, where it passes through n. [By induction: The expression holds for $n = 1$ (where both sides yield 1) and also for $n = 2$ where $1 + x = \frac{1-x^2}{1-x}$. The induction step from n to $n + 1$ is simply $\frac{1-x^n}{1-x} + x^n = \frac{(1-x^n)+(1-x)x^n}{1-x} = \frac{1-x^{n+1}}{1-x}$.]

This can be applied to all the sums with $x = e^{\pm i\frac{\pi}{n+1}(r\pm s)\kappa}$. We just look at the first term individually:

$$\begin{aligned}\sum_{\kappa=1}^{n} e^{i\frac{\pi}{n+1}(r+s)\kappa} &= \sum_{\kappa=0}^{n} e^{i\frac{\pi}{n+1}(r+s)\kappa} - 1 = \frac{1 - e^{i\frac{\pi}{n+1}(r+s)\kappa(n+1)}}{1 - e^{i\frac{\pi}{n+1}(r+s)}} - 1 \\ &= \begin{cases} \frac{1-1}{1-e^{i\frac{\pi}{n+1}(r+s)}} - 1 = -1 & \text{if } r+s \neq 0 \\ n+1-1 & \text{if } r+s = 0 \end{cases} \\ &= \delta_{r,-s}(n+1) - 1 \end{aligned} \tag{1.11.83}$$

All others follow the same pattern. We obtain

$$\begin{aligned}&\sum_{\kappa=1}^{n} \sin(\frac{\pi r}{n+1}\kappa)\sin(\frac{\pi s}{n+1}\kappa) \\ &= -\frac{1}{4}\left((\delta_{r,-s}(n+1)-1) - (\delta_{rs}(n+1)-1) - (\delta_{rs}(n+1)-1) + (\delta_{r,-s}(n+1)-1)\right) \\ &= \frac{n+1}{2}\Big(\delta_{r,s} + \delta_{r,-s}\Big)\end{aligned} \tag{1.11.84}$$

With $r, s \in (1 : n)$, the $\delta_{r,-s}$ term never triggers and thus can be dropped for our applications.

Aside 1.5 – the Dirac comb and the Poisson summation formula:

The Dirac comb is a periodic version of the δ-distribution, and a such, it has discrete Fourier series representation:

$$\delta_\Delta(x) := \sum_{n=-\infty}^{\infty} \delta(x - n\Delta) = \sum_{k=-\infty}^{\infty} c_k e^{2\pi i k x/\Delta} = \frac{1}{\Delta}\sum_{k=-\infty}^{\infty} e^{2\pi i k x/\Delta} \tag{1.11.85}$$

The last equality emerges since the coefficients c_k encounter precisely one δ-peak of the Dirac comb and

$$c_k = \frac{1}{\Delta}\int_a^{a+\Delta} dx \delta_\Delta(x) = \frac{1}{\Delta}\int_a^{a+\Delta} dx \sum_{n=-\infty}^{\infty} \delta(x - n\Delta) = \frac{1}{\Delta} \tag{1.11.86}$$

Any function that falls off fast enough at infinity (a compact support would do, or a Schwartz function for example) can be made periodic over an interval Δ by summing translated copies of it: $s_\Delta(x) := \sum_{n=-\infty}^{\infty} s(x + n\Delta)$, is periodic with period Δ since any shift $s_\Delta(x) \mapsto s_\Delta(x + k\Delta)$ can be compensated for by a shift $n \mapsto n - k$ in the summation index. The conditions on the falloff guarantee that the sum

converges. (This is a nontrivial exercise.)

$$s_\Delta(x) = \sum_{n=-\infty}^{\infty} s(x+n\Delta) = \int \frac{dk}{2\pi} e^{-ikx} \int dy e^{iky} s_\Delta(y) \tag{1.11.87}$$

But, since s_Δ is periodic, the Fourier integral becomes a Fourier sum. fix this

Example 1.7 – the continuum limit, strings on musical instruments:
And indeed, when we interpret $\eta = k\Delta$ then $\lim_{\Delta\to 0} -\frac{4}{\Delta^2}\sin^2(\frac{k\Delta}{2}) = -k^2$.

Example 1.8 – infinite chain with periodic boundary conditions:
Like fixed boundary conditions at points along the chain, periodicity also forces a restriction of the modes entering the spectral sum. The general solution of the homogeneous equation must still be of the form

$$q_\kappa(t) = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi} \left(A^+_\eta e^{i(\eta\kappa+\omega_\eta t)} + A^-_\eta e^{i(\eta\kappa-\omega_\eta t)} \right) \tag{1.11.88}$$

but with the condition that the solutions are periodic in s interval Δ of κ values:

$$q_{\kappa+\Delta}(t) = q_\kappa(t) \qquad \text{for all times } t. \tag{1.11.89}$$

This implies that each mode (labelled by some $\eta \in]-\pi,\pi[$) must satisfy this condition independently since they are *linearly independent*. Thus we have that, for each η

$$A^+_\eta e^{i(\eta(\kappa+n\Delta)+\omega_\eta t)} + A^-_\eta e^{i(\eta(\kappa+n\Delta)-\omega_\eta t)} \stackrel{!}{=} A^+_\eta e^{i(\eta\kappa+\omega_\eta t)} + A^-_\eta e^{i(\eta\kappa-\omega_\eta t)} \tag{1.11.90}$$

It follows that $e^{i\eta(\kappa+n\Delta)} \stackrel{!}{=} e^{i\eta\kappa}$ i.e. only the subset of η with

$$\eta = \eta_r = \frac{2\pi}{\Delta} r \in]-\pi,\pi[\qquad \text{such that } r \in \mathbb{Z}, \text{ i.e. } r \in]-\tfrac{\Delta}{2},\tfrac{\Delta}{2}[\cap\mathbb{Z}. \tag{1.11.91}$$

is admissible.

We can set

$$A^\pm_\eta = \sum_r \delta(\eta-\eta_r)\tilde{A}^\pm_\eta \tag{1.11.92}$$

to obtain

Exercise 1 – the propagator of the infinite chain is real:

Show that the components of the propagator of the infinite chain can be alternatively written as

$$P_{\kappa\lambda}(t-t') = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, \frac{1}{\omega_\eta} a_{\eta\kappa} a^*_{\eta\lambda} \sin\big(\omega_\eta(t-t')\big) = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi}\, \frac{1}{\omega_\eta} \sin\big(\eta(\kappa-\lambda) + \omega_\eta(t-t')\big) \tag{1.11.93}$$

to verify it is indeed real. Is there a more direct way of showing that the expression is real? Why is it important that $\boldsymbol{P}$ be real? *Hint: split the* sin *and change variables* $\eta \to -\eta$ *in one of the terms.*

that's probably too much – should probably insert some discussion about widening Gaussians

Exercise 2 – travelling wave initial conditions?:

Impose initial conditions on the infinte chain that generate left moving travelling wave. Can you represent stable arbitrary shapes?

Exercise 3 – energy expressions for the infinite linear chain:

Show that the formal expression for the potential energy of the linear chain is given by

$$V = \frac{1}{2}\sum_{\kappa\in\mathbb{Z}} mkq_\kappa^2 + mK(q_\kappa - q_{\kappa+1})^2 = m\frac{1}{2}\int_{-\pi}^{\pi} \omega_\eta^2 Q_\eta^*(t) Q_\eta(t) \tag{1.11.94}$$

and thus diagonalized by the eigenmode expansion.

Provide the associated expression for the total energy of the system.

Exercise 4 – restore damping:

Restore damping in the infinite chain and provide expressions for $\boldsymbol{P}$ and $\boldsymbol{G}$ if we add a damping term to the EOMs according to

$$m\ddot{q}_\kappa(t) - mkq_\kappa(t) + i2m\gamma q_\kappa(t) - K((q_{\kappa+1}(t) - q_\kappa(t)) - (q_\kappa(t) - q_{\kappa-1}(t))) = 0 \qquad \kappa \in \mathbb{Z} \tag{1.11.95}$$

Write the general form of the homogeneous solution at time t in terms of initial positions $\boldsymbol{q}(t')$ and $\dot{\boldsymbol{q}}(t')$ at some initial time t'.

Exercise 5 – cross checks on the Green's function expressions:

Perform cross checks on the Green's function expressions in Eq. (1.11.36).

$$\Big(m(\frac{d}{dt})^2 - mk + mK\boldsymbol{D}\Big)\boldsymbol{G}(t-t') = \delta(t-t') \tag{1.11.96}$$

indepedently for both expressions in Eq. (1.11.36). For the second case you will have do demonstrate that $\boldsymbol{P}(t-t')$ is a solution of the homogeneous equation!

Perform the $\tilde{\omega}$ integral to verify that the expressions are equal.

Exercise 6 – a finite open chain:

Imagine a finite open chain without fixed boundary conditions at the endpoints. This means that the first and the last oscillator do *not* appear twice in the potential energies. This leads to a modified $\boldsymbol{D}$ matrix. It takes the form

$$\begin{pmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{pmatrix} \tag{1.11.97}$$

Looks innocent enough. Can you solve it?

Aside 1.6:

Have a look at stackexchange for some first ideas: https://math.stackexchange.com/questions/114048/how-to-diagonalize-infinite-symmetric-banded-matrices and https://qchu.wordpress.com/2009/06/07/the-catalan-numbers-regular-languages-and-orthogonal-polynomials/ by Qiaoc Yuan for more technology.

We can hope to find the eigenvalues if we can understand the structure of the determinant of the banded $n \times n$ matrix

$$A_n(x) := \begin{pmatrix} x & -1 & 0 & 0 & \dots & 0 \\ -1 & x & -1 & 0 & \dots & 0 \\ 0 & -1 & x & -1 & \dots & 0 \\ & & \ddots & \ddots & \ddots & \vdots \\ \dots & \dots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & x & -1 \\ 0 & 0 & 0 & \dots & -1 & x \end{pmatrix} \tag{1.11.98}$$

The characteristic polynomial we seek is then simply given by $\det(\omega^2 A_n(2 - \frac{\Omega^2}{\omega^2}))$.

It is fairly easy to find $q_n(x) := \det(A_n(x))$ for the first few n:

$$q_1(x) = x \ , \qquad q_2(x) = x^2 + 1 \ , \qquad q_3(x) = x^3 - 2x \ , \qquad \dots \tag{1.11.99}$$

Despite the fact that this looks quite irregular, we can in fact get a recursion formula using Laplace's formula for expansion by rows or columns. As a reminder, this formula states that for any $i \in (1:n)$ the determinant of A can be expressed as

$$\det(A) = \sum_{j=1}^{n} A_{ij}(-1)^{i+j} \det(\mathrm{subm}_{ij}(A)) \qquad \text{for any fixed } i \in (1:n) \tag{1.11.100}$$

where $\mathrm{subm}_{ij}(A)$ is the $(n-1)\times(n-1)$ sub-matrix obtained from A by deleting the i-th row and j-th column. Choosing $i = n$, the sum on the right contains precisely two terms

$$\begin{aligned} \det(A_n(x)) &= [A_n(x)]_{n,n-1}(-1)^{n+(n-1)} \det(A_{n-2}(x)) \cdot 1 + [A_n(x)]_{n,n}(-1)^{2n} \det(A_{n-1}(x)) \\ &= -1 \det(A_{n-2}(x)) + x \det(A_{n-1}(x)) \end{aligned} \tag{1.11.101}$$

and we obtain a recursion formula!

The recursion formula is that for Chebychev polynomials of the second kind, $U_n(x)$, if we identify

$$q_n(x) = U_n(x/2) \tag{1.11.102}$$

This has generating functions, both ordinary

$$\sum_{n=0} U_n(x) t^n = \frac{1}{1 - 2tx + t^2} \ , \tag{1.11.103}$$

and exponential

$$\sum_{n=0}^{\infty} U_n(x) \frac{t^n}{n!} = e^{tx} \left(\cosh\left(t\sqrt{x^2-1}\right) + \frac{x}{\sqrt{x^2-1}} \sinh\left(t\sqrt{x^2-1}\right) \right) \ , \tag{1.11.104}$$

and has the trigonometric property that

$$U_{n-1}(\cos(\theta)) \sin(\theta) = \sin(n\theta) \ . \tag{1.11.105}$$

From the latter we conclude that

$$q_n(2\cos(\theta)) = \frac{\sin((n+1)\theta)}{\sin(\theta)} \tag{1.11.106}$$

so that the roots of $q_n(2\cos(\theta))$ are at $\theta = \frac{k\pi}{n+1},$, $k \in (1:n)$, or equivalently that the roots of $q_n(x)$ are at $x = 2\cos(\frac{k\pi}{n+1})$, $k \in (1:n)$.

To map this back onto the eigenvalues we seek, we need to look at $x = 2 - \frac{\omega^2}{\omega^2}$, i.e. we have zeroes where

$$2 - \frac{\Omega^2}{\omega^2} \stackrel{!}{=} 2\cos(\frac{k\pi}{n+1}) \Leftrightarrow \Omega^2 = 2\omega^2\big(1 - \cos(\frac{k\pi}{n+1})\big) = 4\omega^2 \sin^2(\frac{k\pi}{n+1}) \tag{1.11.107}$$

We conclude that the length n chain is non-degenerate, it possesses n distinct eigenvalues given by

$$\Omega_k = 2\omega \sin(\frac{k\pi}{n+1}) \qquad k \in (1:n) \tag{1.11.108}$$

Now we need real eigenvectors of $\omega^2 A_n(2 - \frac{\Omega^2}{\omega^2})$ of the form

$$\boldsymbol{a}_k(t) = \boldsymbol{a}_{k+} e^{i\Omega_k t} + \boldsymbol{a}_{k-} e^{-i\Omega_k t} \tag{1.11.109}$$

subject to the boundary condition $[a_k(t)]_0 = 0$ $[a_k(t)]_{n+1} = 0$

As a function of the discrete position label (treated as a vector index in the above), this operator has oscillating eigenstates This treatment assume an infinite chain with $i \in \mathbb{Z}$. If the chain is finite (we may choose $i \in (1:n)$) we have to truncate the operator at the endpoints, for $i = 1$, there is the $i - 1$ contribution is absent, for $i = n$ the $i + 1$ contribution is not there. Interestingly we can still have eigenfunctions of the form Eq. (**??**), provided we restrict η:

$$(\delta_{2j} - 2\delta_{1j} + 0\delta_{-1j})a_{kj} = \alpha_k e^{i\eta 1}(e^{i\eta} - 2) + \alpha_k^* e^{-i\eta 1}(e^{-i\eta} - 2) \stackrel{!}{=} -2(1 - \cos(\eta))a_{k1} \tag{1.11.110}$$

$$(0\delta_{n+1j} - 2\delta_{nj} + \delta_{n-1j})a_{kj} = \alpha_k e^{i\eta n}(-2 + e^{-i\eta}) + \alpha_k^* e^{-i\eta n}(-2 + e^{+i\eta}) \stackrel{!}{=} -2(1 - \cos(\eta))a_{kn} \tag{1.11.111}$$

The eigenvalue equations in this case read

The values allowed for η are r

Exercise 7 – the diatomic chain with different masses but identical force constants:

Exercise 8 – the diatomic chain with identical masses but different force constants:

This problem for a diatomic chain is based on Kittel Chapter 4, Problem 5. Consider the normal modes of a linear chain, in which the force constants between nearest-neighbor atoms are alternately C_1 and C_2. Let the masses be equal, and let the nearest-neighbor separation be $a/2$. Find $\omega(k)$ at $k = 0$ and $k = \pi/a$. Sketch in the dispersion relation by eye. This problem simulates a crystal of diatomic molecules such as H_2.

Solution:

We will call the alternating force constants C_1 and C_2 . For one type of atoms, the force constant C_1 is on the right and the force constant C_2 is on the left. For the other type of atoms, C_2 is on the right

and C_1 is on the left. The equations of motion for these two sites are

$$M\ddot{u}_s = C_2(v_s - u_s) + C_1(v_{s-1} - u_s) = C_2 v_s + C_1 v_{s-1} - (C_1 + C_2)u_s \tag{1.11.112}$$
$$M\ddot{v}_s = C_2(u_s - v_s) + C_1(u_s + 1 - v_s) = C_2 u_s + C_1 v_s + 1 - (C_1 + C_2)v_s. \tag{1.11.113}$$

Periodic solutions of the form

$$u_s = u\, e^{i(ksa-\omega t)} \text{ and } v_s = v e^{i(ksa-\omega t)}. \tag{1.11.114}$$

$$\begin{pmatrix} C_1 + C_2 - M\omega^2 & -(C_2 + C_1 e^{-ika}) \\ -(C_2 + C_1 e^{+ika}) & C_1 + C_2 - M\omega^2 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} \stackrel{!}{=} \mathbf{0} \tag{1.11.115}$$

The two eigenvalues come out to be

$$M\omega_\pm^2(k) = (C_1 + C_2) \pm (C_1^2 + C_2^2 + 2C_1 C_2 \cos(ka))^{\frac{1}{2}}. \tag{1.11.116}$$

Then at $k = 0$ $\cos(ka) = 1$ so that

$$M\omega_\pm^2(k = 0) = (C_1 + C_2) \pm (C_1^2 + C_2^2 + 2C_1 C_2)^{\frac{1}{2}} = (C_1 + C_2) \pm |C_1 + C_2| \tag{1.11.117}$$

while at $k = \pi/a$ $\cos(ka) = 0$ so that

$$M\omega_\pm^2(k = 0) = (C_1 + C_2) \pm (C_1^2 + C_2^2)^{\frac{1}{2}} \tag{1.11.118}$$

The zero-frequency mode at k = 0 is called the Goldstone mode. Why is that? (What does that have to do with spontaneous symmetry breaking?)

Remark 1.15 – connections and further reading:

There are many, often higher dimensional generalizations of such systems:

- They play a role in the study of crystals and the excitations propagating through them: sound waves and phonons, spin waves and many additional phenomena.

  There it becomes necessary to discuss periodic systems with different masses in elementary cells that then, as a whole, repeat to create the crystals.

- Statistical field theory and lattice gauge theory perform numerical studies of discrectized systems on lattices with periodic boundary conditions.

  Wipf's "Statistical approach to quantum field theory" [12] has beautiful and concise discussion of a time discretized set of coupled harmonic oscillators in Sec. 2.6, simply titled "The harmonic oscillator". Here it is the time derivative that is discretized instead of a spatial derivative (the local excitations are not correlated in space, the chapter deals with what in the jargon is called a "free theory"). Nevertheless, we see the same mathematics at work, with a slight modification of the linear operators that that appear due to the periodic boundary conditions employed.

Any introduction to lattice field theory will have similar discussions, Sec 2 in Heinz Rothe's "Lattice gauge theory: an introduction" [13] gives a good example worth reading for its concise exposition of completeness and orthogonality relations on a periodic lattice.

Lattice field theory also is formulated on a 3 space + 1 time dimensional regular lattice of points, the formulation is rather more economical than this elementary treatment.

Remark 1.16 – a comment on resolution:

Fig. 9 is a perfect place to talk about resolution.



Talk about a force at too high spatial frequency. Probably also needs talking about a force with any frequency!

2 From Newton to Lagrange – systems with constraints

2.1 Degrees of freedom and constraints

The mechanical systems discussed in chapter 1 were envisioned as sets of n-particles systems that were only subject to inter-particle forces with external forces dealt with mostly as an add on.

Consider now a system where the movement of in configuration space, the particles are constrained to fall onto a smooth "surface" (a sub-manifold of $\mathbb{R}^n$, a concept to be explained below in an elementary manner). A bead on a curved wire (think miniature roller coaster) or a planar pendulum would be simple examples.

It should be intuitively clear that a full description of these systems, including the the wire and rod of the pendulum are quite complicated. We would have to take into account the forces the wire or the rod of the pendulum exert on the mass whose movement we want to discern. For more complicated cases, like a set of particles on a (smooth) surface the complications grow quickly to a complexity that prevents us from finding solutions analytically.

The Lagrangian formulation is a formulation that allows us to sidestep this problem and to altogether avoid the need ever calculate the forces that implement the constraint if we are only interested in the motion of the particles themselves. Even the engineer who needs to know the constraint forces (say to make the wire strong enough or the roller coaster withstand the stresses) can deduce these after the fact in a relatively simple manner.

We will now consider several types of constraints, the simplest of which restrict particle movements to sub-manifolds in configuration space.

Reminder 2.1 – sub-manifold and hypersurface of a vector space:

A k-dimensional sub-manifold of an n-dimensional vector space is in essence the generalization of what a two dimensional surface or a line is to 3-dimensional space: a smooth subset which at all points has a well defined vector space of tangents and normals.

In strict parlance, a hypersurface of an n-dimensional vector space is an $n-1$ dimensional sub-manifold, generalizing the notion of a surface in $\mathbb{R}^3$. Often both terms are used interchangeably.

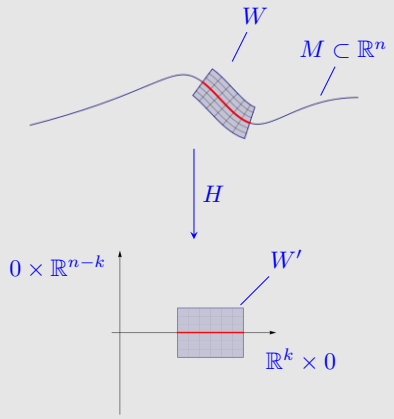
Here we are intrested in sub-manifolds of configuration and/or phase space.

Concepts 2.1 – sub-manifolds of $\mathbb{R}^n$:

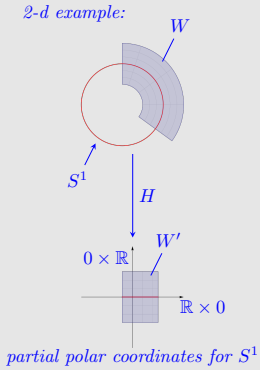
A subset $M \subset \mathbb{R}^n$ is called a k-dimensional sub-manifold or a k-dimensional hypersurface, if for every point $p \in M$, there is an open set $W \subset \mathbb{R}^n$ around it and a diffeomorphism $H : W \xrightarrow{\cong} W'$ such that

$$H(M \cap W) = (\mathbb{R}^k \times 0) \cap W'$$

Pictorially:



$M \cap W$ and its image are marked in red



partial polar coordinates for S^1

In words: what H does is to "straighten out" M in terms of coordinates. Compare this with the remarks about curvilinar coordinate systems near Eq. (1.2.18) and consult App. B.1.1 for additional background material on manifolds in general.

Constraints to sub-manifolds in configuration space $\mathfrak{C} = \mathbb{R}^{3n}$ or *holonomic* constraints:

Envision a system of n particles that is subject to k-conditions of a form that involves only particle coordinates

$$f^I(\boldsymbol{x}, t) = 0 \qquad I = 1, \ldots, k < 3n, \qquad \boldsymbol{x} := \begin{pmatrix} \boldsymbol{r}_1 \\ \vdots \\ \boldsymbol{r}_n \end{pmatrix} \in \mathfrak{C} = \mathbb{R}^{3n} \tag{2.1.1}$$

Constraints of this type are called *holonomic* (meaning essentially integrable in Greek).

The f^I are assumed to be differentiable and the t dependence describes the way the constraint changes over time in a way that is independent of the position of the particles (imagine for example that we rattle the wire or the pendulum in a prescribed way). A famous example of a time dependent constraint is Foucault's pendulum – any pendulum forced to move with the surface of the earth as it rotates around its polar axis.

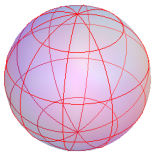
Each one of these conditions is capable of imposing exactly one restriction on the configuration space coordinate $\boldsymbol{x}$ and thus may reduce the "dimensionality" of the allowed configuration space (at most) by one.

To ensure that we get *exactly* one res is indeed happening we need to ensure that the f^I are independent in a suitable way to be defined below.

The subspaces of configuration space selected in this way are in fact sub-manifolds of $\mathfrak{C} = \mathbb{R}^{3n}$

Examples of holonomic constraints and associated submanifolds of $\mathfrak{C} = \mathbb{R}^{3n}$:

- The constraint surface of a (non-planar) pendulum is S^2, the two dimensional sphere, we have $n = 1$ and $k = 1$:



$$f(\boldsymbol{r}) = \boldsymbol{r}^2 - r_0^2 = 0$$

- Patch of an infinitely extended two dimensional constraint surface: $n = 1, k = 1$

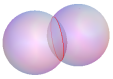


$$f(\boldsymbol{r}) = \frac{x^2 - y^2}{10} - z = 0$$

- Combining two independent conditions reduces the dimensionality of the constraint manifold further $n = 1, k = 2$:

$$f^1(\boldsymbol{r}) = \frac{y^2 - x^2}{10} - z = 0;$$
$$f^2(\boldsymbol{r}) = \frac{y^2 - z^2}{10} - x = 0.$$

- Here is a circle from two spherical constraints, again $n = 1, k = 2$:



$$f^1(\boldsymbol{r}) = \boldsymbol{r}^2 - 1 = 0;$$
$$f^2(\boldsymbol{r}) = (\boldsymbol{r} + \hat{\boldsymbol{e}}_1 + \hat{\boldsymbol{e}}_2)^2 - 1 = 0$$

Note that the constraint functions are not unique: we may arrive at the same constraint manifold by requiring

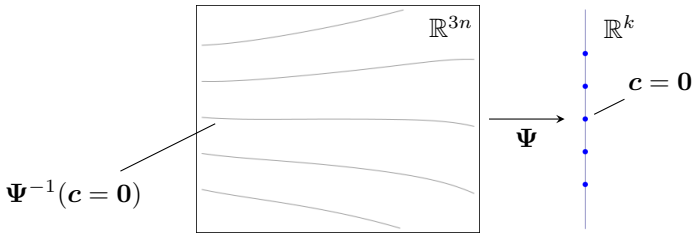
$$f^1(\boldsymbol{r}) = \boldsymbol{r}^2 - 1 = 0;$$
$$f^2(\boldsymbol{r}) = \boldsymbol{r} \cdot (\hat{\boldsymbol{e}}_1 + \hat{\boldsymbol{e}}_2) - 1 = 0$$

which selects the intersection of a sphere with a plane.

Let us think of the f^I as components of a vector valued map on configuration space (for each t):

$$\begin{aligned} &\Psi_t : \mathbb{R}^{3n} \to \mathbb{R}^k \\ &\boldsymbol{x} \mapsto \Psi(\boldsymbol{x}, t) := \begin{pmatrix} f^1(\boldsymbol{x}, t) \\ \vdots \\ f^k(\boldsymbol{x}, t) \end{pmatrix} \end{aligned} \tag{2.1.2}$$

then, in the above construction we are looking for the *levels* of this map in configuration space $\mathbb{R}^{3n}$, i.e. the subsets $\Psi_t^{-1}(c) \subset \mathbb{R}^{3n}$ that map onto a fixed point $c \in \mathbb{R}^k$:

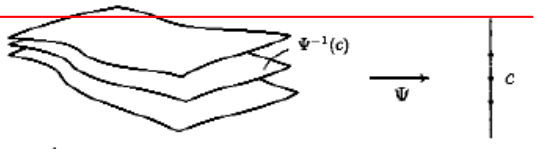


Schematic view of the levels of the constraint map

This picture is very schematic, the dimensionality of the level sets will crucially depend on k. I can show the generic examples for $3n = 3$:

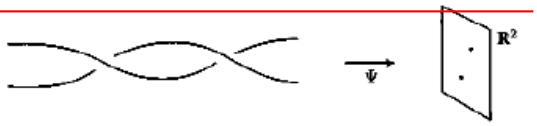
Fix Graphics

- $n = 1$ and $k = 1$, the level sets are two dimensional hypersurfaces of $\mathbb{R}^3$, surfaces in the usual sense



Fix Graphics

- $n = 1$ and $k = 2$, the level sets are one dimensional hypersurfaces, i.e. lines



› **General *non-holonomic* constraints:**

Constraints that can not be cast in the form (2.1.1) are called *non-holonomic*.

- **Non-holonomic constraints to sub-manifolds of phase-space:** These are constraints that follow the general pattern of holonomic constraints, but also depend on velocities (rolling constraints, say for a wheel on a surface among them).

$$f^I(\boldsymbol{x}, t) = 0 \qquad I = 1, \ldots, k < 3n, \qquad \boldsymbol{x} := \begin{pmatrix} \boldsymbol{r}_1 \\ \vdots \\ \boldsymbol{r}_n \\ \boldsymbol{p}_1 \\ \vdots \\ \boldsymbol{p}_n \end{pmatrix} \in \mathfrak{P} = \mathbb{R}^{6n} \tag{2.1.3}$$

  One may view holonomic constraints as a special case of these.

- **Non-holonomic constraints that do not correspond to a sub-manifold of phase space:**
  These are often given by inequalities, be it on configuration space (i.e. particle coordinates: think particles confined to a box) or on phase space.
  Such subspaces can usually not be thought of as sub-manifolds (the notion of tangent and normal vectors at each point in the subspace is lacking).

› **Do the constraints depend on time explicitly?**

One distinguishes constraints with an explicit time dependence, *rheonomic* ("running law") constraints and such without, *scleronomic* ("rigid law") constraints.

In the following we will focus on holonomic constraints, constraints to sub-manifolds of configuration space. Keep in mind, however, that a generalization to the case of a general sub-manifold in phase space is conceptually not hard.

Imagine a situation in which

$$\dot{\boldsymbol{p}} = m\ddot{\boldsymbol{x}} = \boldsymbol{F} + \boldsymbol{C} \tag{2.1.4}$$

where

$$\boldsymbol{x} = \begin{pmatrix} \boldsymbol{r}_1 \\ \vdots \\ \boldsymbol{r}_n \end{pmatrix}, \ \boldsymbol{F} = \begin{pmatrix} \boldsymbol{F}_1 \\ \vdots \\ \boldsymbol{F}_n \end{pmatrix}, \ \boldsymbol{C} = \begin{pmatrix} \boldsymbol{C}_1 \\ \vdots \\ \boldsymbol{C}_n \end{pmatrix} \in \mathbb{R}^{3n} \tag{2.1.5}$$

represent trajectories in the configuration space of an n-particle system and forces acting on them respectively.

I particular, we want $\boldsymbol{C}$ to represent the forces of constraint, the forces that keep the particles on the hypersurface of $\mathbb{R}^{3n}$, while $\boldsymbol{F}$ will describe the dynamics inside the hypersurface allowed by the constraint. To achieve this $\boldsymbol{C}$ *must be perpendicular* to the hypersurface, $\boldsymbol{F}$ must be tangential to it!

To construct a suitable $\boldsymbol{C}$ one needs to know what direction is orthogonal to the hypersurface (this gives the direction of the force) and, in the end, the amplitude at each point on the hypersurface at each time. Sounds formidable!

All we know at this point is the set of constraint equations (2.1.1), which now read

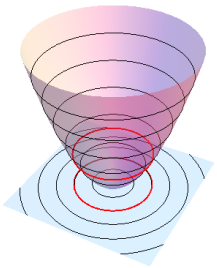
$$f^I(\boldsymbol{x}, t) = 0 \quad I = 1, \ldots, k < 3n \tag{2.1.6}$$

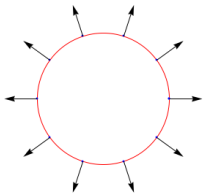
k must be smaller than $3n$, so that motion is possible at all.

Note, however, that

$$\boldsymbol{\nabla}_{\boldsymbol{x}} f^I(\boldsymbol{x}, t) \in \mathbb{R}^{3n} \quad \forall \ I == 1, \ldots, k < 3n \tag{2.1.7}$$

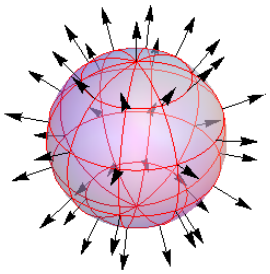
(if nonzero) is automatically perpendicular to the hypersurface defined by (2.1.6).

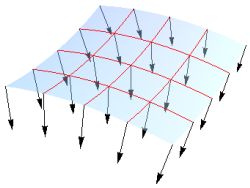


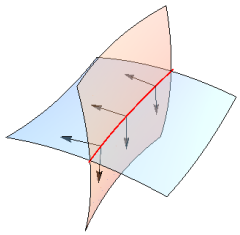


Consider a 2-d problem with constraint $f(\boldsymbol{r}) = \boldsymbol{r}^2 - c = 0$. (This is akin to looking at a harmonic oscillator potential and selecting the potential value $2c/(m\omega^2)$.) We know that the (two dimensional gradient) is perpendicular to the contour lines of the function we differentiate, after all (and up to a minus sign), this is how we calculate the force induced by the potential.

Likewise for the other examples:







If $\boldsymbol{\nabla}_{\boldsymbol{x}} f^I(\boldsymbol{x}, t) \neq \boldsymbol{0}$ on $f^I(\boldsymbol{x}, t) = 0$, then we have the desired normal direction!

- **Remarks:**
  - $\boldsymbol{\nabla}_{\boldsymbol{x}} f^I(\boldsymbol{x},t) \neq \boldsymbol{0}$ on $f^I(\boldsymbol{x},t) = 0$ can always be achieved by a suitable choice of constraint function altough this is not automatic:
    For example the equations $f(\boldsymbol{x}) = \boldsymbol{s}\cdot\boldsymbol{x} = 0$ and $f(\boldsymbol{x}) = (\boldsymbol{s}\cdot\boldsymbol{x})^2 = 0$ both constrain the system to the same plane (through the origin and perpendicular to $\boldsymbol{s}$ so that $\boldsymbol{s}\cdot\boldsymbol{x} = 0$), but only the first leads to a nonvanishing gradient on that plane.
  - Since the constraint functions only define the geometry of the constraint sub-manifold this construction can only provide us with the *direction* of the constraint force, which is a *kinematical* piece of information.
    The *magnitude* of the constraint force is a *dynamical* quantity: The centrifugal force a pendulum rod must compensate for depends on the velocity of the pendulum and can thus only be obtained after we know the full dynamical solutions to the problem.

If $k = 1$, this construction leads to a force of constraint that must be of the form

$$\boldsymbol{C} = \lambda(t)\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x},t)$$

where $\lambda(t)$ parametrizes the amplitude of the force.

This is the content of the theorem of implicit functions, more below.

If the number of constraints k is larger than one, we observe that

- the $\boldsymbol{\nabla}_{\boldsymbol{x}} f^I(\boldsymbol{x},t)$ must span the space normal to the sub-manifold at $\boldsymbol{x}$ and t.
  This is in fact a *prerequisite* for the $f^I(\boldsymbol{x},t) = 0$ to define a sub-manifold of $\mathbb{R}^{6n}$.
- Its complement in $\mathbb{R}^{3n}$ is tangent to the hypersurface at $\boldsymbol{x}$ and t, for which we can also choose a basis of vectors

  $$\{\delta\boldsymbol{x}^\alpha : 1,\dots,3n-k\} \tag{2.1.8}$$

  $3n-k$ is the dimension of the constraint hypersurface or manifold and gives the number of degrees of freedom after the constraints have been taken into account:

  $$f = 3n-k\ . \tag{2.1.9}$$

Altogether we have constructed a basis for configuration space $\mathfrak{C}$ in the form

$$\{\delta\boldsymbol{x}^1,\dots,\delta\boldsymbol{x}^{3n-k}, \boldsymbol{\nabla}_{\boldsymbol{x}} f^1(\boldsymbol{x},t),\dots \boldsymbol{\nabla}_{\boldsymbol{x}} f^k(\boldsymbol{x},t)\} \tag{2.1.10}$$

which is not orthonormal. What is important is that it constitutes a basis, a complete set of linearly independent vectors and that

$$\delta\boldsymbol{x}^\alpha \cdot \nabla_{\boldsymbol{x}} f^I(\boldsymbol{x},t) = 0 \qquad \text{for all } \alpha = 1,\dots,f = 3n-k \text{ and } I = 1,\dots,k. \tag{2.1.11}$$

2.2 d'Alembert's principle and the derivation of Lagrange's equation

From the fact that the $\boldsymbol{\nabla}_{\boldsymbol{x}} f^I$ span the space normal to the constraint surface we conclude that we may expand the constraint force in terms of the $\boldsymbol{\nabla}_{\boldsymbol{x}} f^I(\boldsymbol{x},t)$:

$$\boldsymbol{C} = \sum_{I=1}^{k} \lambda^I(t)\boldsymbol{\nabla}_{\boldsymbol{x}} f^I(\boldsymbol{x},t) \tag{2.2.1}$$

and the coupled set of equations we need to solve (Eq (2.1.4)) turns into

$$\dot{\boldsymbol{p}} - \boldsymbol{F} - \sum_{I=1}^{k} \lambda^I(t) \boldsymbol{\nabla}_{\boldsymbol{x}} f^I(\boldsymbol{x}, t) = 0 \tag{2.2.2a}$$

$$f^I(\boldsymbol{x}, t) = 0 \quad I = 1, \ldots, k < 3n \tag{2.2.2b}$$

Recall that $(\dot{\boldsymbol{p}} - \boldsymbol{F})$ and $\delta\boldsymbol{x}^\alpha \in \mathfrak{C}$ for each α!

Projecting this relation onto any of the $\delta\boldsymbol{x}^\alpha$ and using Eq. (2.1.11) we conclude that

$$(\dot{\boldsymbol{p}} - \boldsymbol{F}) \cdot \delta\boldsymbol{x}^\alpha = 0 \qquad \text{for all } \alpha = 1, \ldots, 3n - k. \tag{2.2.3}$$

This equation is usually called d'Alembert's principle, the basis elements $\delta\boldsymbol{x}^\alpha$ are referred to as virtual displacements, directions of movement which are locally (at $\boldsymbol{x}$ and t) allowed by the constraint equations. Again these are the directions tangent to the constraint manifolds.

We now embark on constructing a suitable set of (generally curvilinear) coordinates, i.e. a set of invertible functions of the components x^i of $\boldsymbol{x}$:

$$q^\alpha(x^1, \ldots, x^{3n}, t), \quad \alpha = 1, \ldots, 3n \tag{2.2.4}$$

so that we can reconstruct the x^β from them

$$x^\beta(q^1, \ldots, q^{3n}, t), \quad \beta = 1, \ldots, 3n \tag{2.2.5}$$

which also are twice continuously differentiable to be able to represent accelerations also in terms of the q^α.

Remark 2.1 – invertibility = non-singular Jacobian:
Invertibility means that the Jacobian matrix $\frac{\partial q^\alpha}{\partial x^\beta}$ of the transformation be nonsingular: $\det[\frac{\partial q^\alpha}{\partial x^\beta}] \neq 0$ locally, i.e. in an open set around a solution $\boldsymbol{x}_0$ to the constraint equations $f^I(\boldsymbol{x}, t) = 0$.

While locally such functions can always be found, there are sets of generalized coordinates which are especially suited for our purpose: Imagine a set of q^α which on the constraint sub-manifold have

$$\{\delta\boldsymbol{x}^1, \ldots, \delta\boldsymbol{x}^{3n-k}, \boldsymbol{\nabla}_{\boldsymbol{x}} f^1(\boldsymbol{x}, t), \ldots \boldsymbol{\nabla}_{\boldsymbol{x}} f^k(\boldsymbol{x}, t)\} \tag{2.2.6}$$

as their tangent vectors:

$$\delta\boldsymbol{x}^\alpha = \frac{\partial \boldsymbol{x}}{\partial q^\alpha} \in \mathfrak{C} \qquad \text{for } \alpha = 1, \ldots, f = 3n - k \tag{2.2.7}$$

$$\boldsymbol{\nabla}_{\boldsymbol{x}} f^I(\boldsymbol{x}, t) = \frac{\partial \boldsymbol{x}}{\partial q^{f+I}} \in \mathfrak{C} \qquad \text{for } I = 1, \ldots, k \tag{2.2.8}$$

locally, i.e. in an open set around a solution $\boldsymbol{x}_0$ to the constraint equations $f^I(\boldsymbol{x}, t) = 0$.

Warning 2.1 – useful generalized coordinates will generally not exist globally:
Note that there is no reason that such coordinate systems will exist globally i.e. for all points in $\mathfrak{C}$ (or $\mathfrak{P}$).

Generically, we will need to be prepared to have different sets of coordinates on open sets U_i that cover the constraint manifold, along with the requirement that change of coordinates $U \cap U' \to U \cap U', q^\alpha \mapsto$

$q'^{\alpha}(q^{\beta},t)$ is locally smooth and invertible $\det \frac{\partial q^{\alpha}}{\partial q'^{\beta}} \neq 0$

Eq. (2.2.8) implies that the last k of them $q^{f+I} = q^{3n-k}, \ldots, q^{3n}$ remain constant as the particle moves in the constraint sub-manifold: they decouple from the equations of motion (2.2.3).

An equivalent statement would be that the q^{f+I} can be written purely as functions R^I of the constraint functions f^I:

$$q^{f+I} = R^I(f^1(\boldsymbol{x},t),\ldots,f^k(\boldsymbol{x},t)), \quad I = 1,\ldots,k \tag{2.2.9}$$

or equivalently the f^I must be expressible in terms of the q^{f+I} alone.

The *dynamics*, the nontrivial part of the information encoded in Newton's laws, are represented by d'Alembert's principle, Eq. (2.2.3), is now purely encoded in the first f coordinates with $\delta\boldsymbol{x}^{\alpha} = \frac{\partial \boldsymbol{x}}{\partial q^{\alpha}} \in \mathfrak{C}$.

This is the first step towards translating d'Alembert's principle, the EOM's, into our new set of coordinates.

› **step 1 – insert virtual displacements:** d'Alembert's equation now reads

$$(\dot{\boldsymbol{p}} - \boldsymbol{F}) \cdot \frac{\partial \boldsymbol{x}}{\partial q^{\alpha}} = 0 \qquad \text{for all } \alpha = 1,\ldots,3n-k. \tag{2.2.10}$$

› **step 2 – rewrite force term:** The force term defines a generalized force:

$$Q^{\alpha} := \boldsymbol{F} \cdot \frac{\partial \boldsymbol{x}}{\partial q^{\alpha}} \tag{2.2.11}$$

If we assume that $\boldsymbol{F}$ is conservative also the generalized force is conservative:

$$\boldsymbol{F} \cdot \frac{\partial \boldsymbol{x}}{\partial q^{\alpha}} = -(\boldsymbol{\nabla}_{\boldsymbol{x}} U) \cdot \frac{\partial \boldsymbol{x}}{\partial q^{\alpha}} = -\frac{\partial U}{\partial q^{\alpha}} \tag{2.2.12}$$

Let me split a generic force into a conservative and a non-conservative part Q^{α}_{nc} and write

$$\boldsymbol{F} \cdot \frac{\partial \boldsymbol{x}}{\partial q^{\alpha}} = -\frac{\partial U}{\partial q^{\alpha}} + Q^{\alpha}_{\text{nc}} \tag{2.2.13}$$

› **step 3 – replace $\dot{p}$:**

$$\dot{\boldsymbol{p}} \cdot \frac{\partial \boldsymbol{x}}{\partial q^{\alpha}} = \frac{d}{dt}\left[\boldsymbol{p} \cdot \frac{\partial \boldsymbol{x}}{\partial q^{\alpha}}\right] - \boldsymbol{p} \cdot \frac{d}{dt}\frac{\partial \boldsymbol{x}}{\partial q^{\alpha}} \tag{2.2.14}$$

For holonomic constraints

$$f^I(\boldsymbol{x},t) = f^I(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_n,t) = 0 \tag{2.2.15}$$

(independent of the $\dot{\boldsymbol{r}}_i$) we can solve locally for the coordinates that satisfy the constraint (2.2.15) withouth involving the velocities $\dot{\boldsymbol{r}}_i$ and $\dot{q}^{\alpha}$

$$\boldsymbol{x} = \boldsymbol{x}(q^1,\ldots,q^{3n},t) \tag{2.2.16}$$

In particular

$$\frac{\partial \boldsymbol{x}}{\partial \dot{q}^{\alpha}} = 0 \tag{2.2.17}$$

for coordinates that satisfy the constraints.

[In fact we can solve locally for the coordinates that satisfy the constraint (2.2.15) in terms of the first f of the q^α (q^1 through q^f) alone.]

Eq. (2.2.15) allows to simplify chain rule expressions like (summation convention on α!)

$$\boldsymbol{v} := \dot{\boldsymbol{x}} = \frac{d\boldsymbol{x}}{dt} = \frac{\partial \boldsymbol{x}}{\partial q^\alpha}\dot{q}^\alpha + \underbrace{\frac{\partial \boldsymbol{x}}{\partial \dot{q}^\alpha}}_{=0}\ddot{q}^\alpha + \frac{\partial \boldsymbol{x}}{\partial t} = \frac{\partial \boldsymbol{x}}{\partial q^\alpha}\dot{q}^\alpha + \frac{\partial \boldsymbol{x}}{\partial t} \tag{2.2.18}$$

Together with (2.2.17) this states that $\boldsymbol{v}$ is at most linear in $\dot{q}^\alpha$, the coefficient of that linear term is $\frac{\partial \boldsymbol{x}}{\partial q^\alpha}$. An immediate consequence of this is that for $\boldsymbol{x}$ that satisfy the constraint

$$\frac{\partial \boldsymbol{v}}{\partial \dot{q}^\alpha} = \frac{\partial \dot{\boldsymbol{x}}}{\partial \dot{q}^\alpha} = \frac{\partial \boldsymbol{x}}{\partial q^\alpha} \tag{2.2.19}$$

which is often referred to as the cancellation of dots. This allows us to read the first term in Eq. (2.2.14) as

$$\frac{d}{dt}\left[\boldsymbol{p}\cdot\frac{\partial \boldsymbol{x}}{\partial q^\alpha}\right] = \frac{d}{dt}\left[\boldsymbol{p}\cdot\frac{\partial \dot{\boldsymbol{x}}}{\partial \dot{q}^\alpha}\right] \ . \tag{2.2.20}$$

$\frac{\partial \boldsymbol{x}}{\partial \dot{q}^\alpha} = 0$ also helps to rewrite the second term in Eq. (2.2.14), in which

$$\frac{d}{dt}\frac{\partial \boldsymbol{x}}{\partial q^\alpha} = \frac{\partial^2 \boldsymbol{x}}{\partial q^\alpha \partial q^\beta}\dot{q}^\beta + \frac{\partial}{\partial t}\frac{\partial \boldsymbol{x}}{\partial q^\alpha} = \frac{\partial}{\partial q^\alpha}\underbrace{\left(\frac{\partial \boldsymbol{x}}{\partial q^\beta}\dot{q}^\beta + \frac{\partial \boldsymbol{x}}{\partial t}\right)}_{\frac{d\boldsymbol{x}}{dt}} = \frac{\partial}{\partial q^\alpha}\frac{d\boldsymbol{x}}{dt} = \frac{\partial \boldsymbol{v}}{\partial q^\alpha} \tag{2.2.21}$$

We now have

$$(2.2.14) = \frac{d}{dt}\left[\boldsymbol{p}\cdot\frac{\partial \boldsymbol{v}}{\partial \dot{q}^\alpha}\right] - \boldsymbol{p}\cdot\frac{\partial \boldsymbol{v}}{\partial q^\alpha} \tag{2.2.22}$$

To proceed, we unravel the sum over particles inside this:

$$\begin{aligned} &= \sum_i \left\{\frac{d}{dt}\left[\boldsymbol{p}_i\cdot\frac{\partial \boldsymbol{p}_i/m_i}{\partial \dot{q}^\alpha}\right] - \boldsymbol{p}_i\cdot\frac{\partial \boldsymbol{p}_i/m_i}{\partial q^\alpha}\right\} = \sum_i \left\{\frac{d}{dt}\frac{\partial}{\partial \dot{q}^\alpha}\frac{\boldsymbol{p}_i^2}{2m_i} - \frac{\partial}{\partial q^\alpha}\frac{\boldsymbol{p}_i^2}{2m_i}\right\} \\ &= \frac{d}{dt}\frac{\partial T}{\partial \dot{q}^\alpha} - \frac{\partial T}{\partial q^\alpha} \qquad T := \sum_i \frac{\boldsymbol{p}_i^2}{2m_i} \end{aligned} \tag{2.2.23}$$

We have arrived at

$$\frac{d}{dt}\frac{\partial T}{\partial \dot{q}^\alpha} - \frac{\partial T}{\partial q^\alpha} + \frac{\partial U}{\partial q^\alpha} = Q^\alpha_{\text{nc}}$$

were the Q^α_{nc} stand for any nonconservative part of the generalized forces.

Since $\frac{\partial U}{\partial \dot{q}^\alpha} = 0$, we may state this in terms of the *Lagrangian* (function)

$$L := T - U \tag{2.2.24}$$

as

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^\alpha} - \frac{\partial L}{\partial q^\alpha} = Q^\alpha_{\rm nc} \qquad \alpha = 1, \ldots, f = 3n - k \tag{2.2.25}$$

If there are no non-conservative forces acting on the system, we have

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^\alpha} - \frac{\partial L}{\partial q^\alpha} = 0 \qquad \alpha = 1, \ldots, f = 3n - k \tag{2.2.26}$$

These are simply a restatement of Newton's laws that allow to choose coordinates in a way that eliminates constraints on the degrees of freedom completely. Without constraints we recover the original formulation in whatever set of coordinates we wish to choose.

› From Wikipedia (*much more there*): Joseph-Louis Lagrange (25 January 1736 – 10 April 1813), born Giuseppe Luigi Lagrancia (often known as Giuseppe Luigi Lagrangia in the scientific literature) was an Italian-born French mathematician and astronomer born in Turin, Piedmont, who lived part of his life in Prussia and part in France. He made significant contributions to all fields of analysis, number theory, and classical and celestial mechanics. On the recommendation of Euler and d'Alembert, in 1766 Lagrange succeeded Euler as the director of mathematics at the Prussian Academy of Sciences in Berlin, where he stayed for over twenty years, producing a large body of work and winning several prizes of the French Academy of Sciences. Lagrange's treatise on analytical mechanics (Mécanique Analytique, 4. ed., 2 vols. Paris: Gauthier-Villars et fils, 1888–89), written in Berlin and first published in 1788, offered the most comprehensive treatment of classical mechanics since Newton and formed a basis for the development of mathematical physics in the nineteenth century.



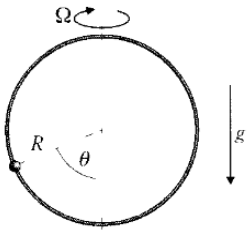
The equations (2.2.25) indeed form a set of second order equations for the q^α as can be seen by applying the chain rule for the explicit time derivative:

$$Q^\alpha_{\rm nc} = \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^\alpha} - \frac{\partial L}{\partial q^\alpha} = \frac{\partial^2 L}{\partial \dot{q}^\alpha \partial \dot{q}^\beta}\ddot{q}^\beta + \frac{\partial^2 L}{\partial \dot{q}^\alpha \partial q^\beta}\dot{q}^\beta + \frac{\partial^2 L}{\partial \dot{q}^\alpha \partial t} - \frac{\partial L}{\partial q^\alpha}$$

› **Remark 2.2 – this much from mere existence?:**
Note that in order to derive Lagrange equations we have only needed existence statements for the type of coordinate system we seek. These are needed to ensure the formal manipulations performed to arrive at Lagrange's equations (2.2.25) are guaranteed to work.

How useful is such a result? How much mileage do we get? This is best answered by analyzing an example that has a constraint that is more complicated than a mere pendulum:

› **Example – Bead on a vertical rotating hoop:**
A bead of mass m slides without friction in a uniform gravitational field on a vertical circular hoop of radius R. The hoop is constrained to rotate at a fixed angular velocity Ω about its vertical diameter. Let θ be the position of the bead on the hoop measured from the lowest point.



Fix Graphics

- Write down the Lagrangian $L(\theta, \dot{\theta})$
- Find how the equilibrium values of θ depend on Ω. Which are stable, which unstable?
- Find the frequencies of small vibrations about the stable equilibrium positions. What can you say about the motion around the only stable equilibrium point when $\Omega = \sqrt{g/R}$?

Solution:

- Spherical coordinates r, θ, φ are the coordinates of choice, since there the constraints are manifestly simplest:

$$r = R; \qquad \varphi = \Omega t \tag{2.2.27}$$

(We choose to interpret the second one as an explicitly time dependent constraint on configuration space!)

The configuration manifold remains 1-d ($f = 3-2 = 1$), the single remaining dynamical variable is $\theta(t)$. The potential is simply $U = -mgR\cos\theta$ and only the kinetic term needs a little work. Recall from tutorial 1 that

$$\hat{\boldsymbol{e}}_r = \hat{\boldsymbol{e}}_x \sin\theta\cos\varphi + \hat{\boldsymbol{e}}_y \sin\theta\sin\varphi + \hat{\boldsymbol{e}}_z\cos\theta \tag{2.2.28}$$
$$\hat{\boldsymbol{e}}_\varphi = -\hat{\boldsymbol{e}}_x \sin\varphi + \hat{\boldsymbol{e}}_y\cos\varphi \tag{2.2.29}$$
$$\hat{\boldsymbol{e}}_\theta = \hat{\boldsymbol{e}}_x \cos\theta\cos\varphi + \hat{\boldsymbol{e}}_y \cos\theta\sin\varphi - \hat{\boldsymbol{e}}_z\sin\theta \tag{2.2.30}$$

so that

$$\boldsymbol{v} = \dot{r}\hat{\boldsymbol{e}}_r + r\dot{\hat{\boldsymbol{e}}}_r = \dot{r}\hat{\boldsymbol{e}}_r + r(\dot{\theta}\hat{\boldsymbol{e}}_\theta + \dot{\varphi}\sin\varphi\hat{\boldsymbol{e}}_\varphi) \tag{2.2.31}$$

and

$$\boldsymbol{v}^2 = \dot{r}^2 + r^2(\dot{\theta}^2 + \dot{\varphi}^2\sin^2\theta)\ . \tag{2.2.32}$$

Inserting the constraints yields

$$T = \frac{1}{2}mR^2(\dot{\theta}^2 + \Omega^2\sin^2\theta) \tag{2.2.33}$$

and

$$L = \frac{1}{2}mR^2(\dot{\theta}^2 + \Omega^2\sin^2\theta) + mgR\cos\theta \tag{2.2.34}$$

It is useful to reinterpret this in terms of an effective kinetic and potential energy according to

$$T_{\text{eff}} := \frac{1}{2} mR^2 \dot{\theta}^2 \qquad \text{and} \qquad U_{\text{eff}} := mgR\Big(\frac{1}{2}\frac{\Omega^2}{g/R}\cos^2\theta - \cos\theta + 1\Big) \tag{2.2.35}$$

In writing U_{eff} in this form, I have used the fact that it is determined up to an integration constant (independent of θ) which here is chosen such that U_{eff} at $\theta = 0$ is zero if the loop is not rotating ($\Omega = 0$). The form

$$\tilde{U}_{\text{eff}} := -\frac{1}{2} mR^2\Omega^2 \sin^2\theta - mgR\cos\theta \tag{2.2.36}$$

that is directly suggested by Eq. (2.2.34) would equally be a valid choice – the two versions differ by a term that is independent of θ but does depend on $a = \frac{\Omega^2}{g/R}$ (recall that $\cos^2\theta = 1 - \sin^2\theta$ to see this). All information about fixed points extracted analytically below can be read off qualitatively from the plots of U_{eff} in Fig. 11.

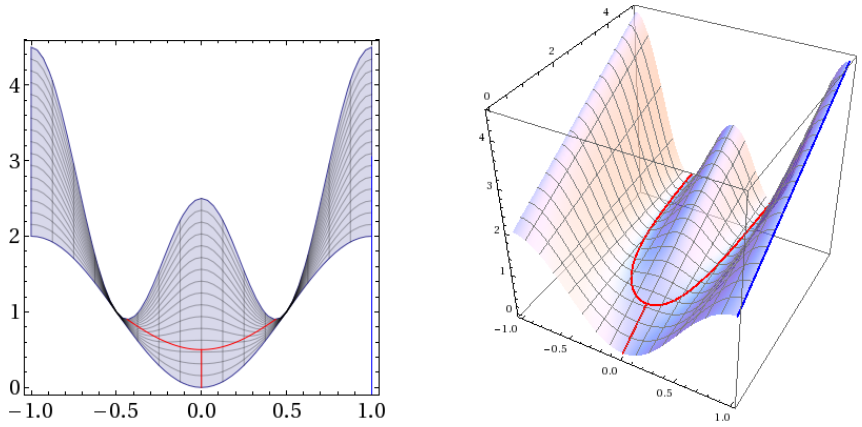


Fig. 11: *Left: $U_{\text{eff}}/(mgR)$ for the rotating pendulum against θ/π for $0 \le \frac{\Omega^2}{g/R} \le 5$. The stability of extrema (stable ones marked in red, unstable ones in blue) can be read off by eye. Right: 3-d plot of same, the left is the view "inwards from the front" of this.*

- To find the equilibrium values (fixed points) we need the EOM and find its stationary points:
  The EOM (divided by mR^2) reads

$$\ddot{\theta} = \Omega^2 \sin\theta\cos\theta - \frac{g}{R}\sin\theta = (\Omega^2\cos\theta - \frac{g}{R})\sin\theta =: F(\theta) = -\frac{1}{mR^2}\frac{\partial}{\partial\theta}U_{\text{eff}}(\theta) \tag{2.2.37}$$

  This latter identification justifies the introduction of T_{eff} and U_{eff} above.
  The equilibrium occurs where the force vanishes, i.e. at $\theta = 0, \pi$ (where $\sin\theta$ vanishes) and at the solution to

$$\cos\theta_0 \stackrel{!}{=} \frac{g}{R\Omega^2} \tag{2.2.38}$$

  The latter only has solutions for $\Omega \ge \sqrt{g/R}$ where the r.h.s. does not exeed one. As Ω approaches $\sqrt{g/R}$ from above this merges with $\theta = 0$. As Ω increases towards infinity, $\theta_0 \to \pi/2$.

To check on stability, read $F(\theta) = -\partial_\theta U(\theta)$ and take a further θ-derivative on the force to check the sign: We need to check if $\partial_\theta^2 U(\theta)$ is positive at $\theta = \pi, \theta_0, 0$. The expression to check is

$$\frac{\partial_\theta^2 U(\theta)}{mgR} = \frac{g}{R}\Big(\frac{\Omega^2}{g/R}(\sin^2\theta - \cos^2\theta) + \cos\theta\Big) \tag{2.2.39}$$

so that we find (compare this to Fig. 11)

- $\theta = \pi$ is obviously unstable
- θ_0 is stable for $\theta_0 \in]0, \pi/2[$, in the whole possible range (for $\frac{g}{R\Omega^2} < 1$ or $\Omega > \sqrt{g/R}$).
- $\theta = 0$ is stable for $1 < \frac{g}{R\Omega^2}$ and unstable otherwise. At $\frac{g}{R\Omega^2}$ the stable point bifurcates into the two possible solutions of $\cos\theta_0 \overset{!}{=} \frac{g}{R\Omega^2}$ at positive and negative θ_0. See also Fig. 11
- For $\Omega > \sqrt{g/R}$, the first term in a Taylor series expansion of the Force in the EOM about θ_0 yields

  $$\ddot\theta = -(\theta - \theta_0)\Omega^2 \sin^2\theta_0 + \mathcal{O}(\theta^2) = -(\theta - \theta_0)\Omega^2(1 - (\tfrac{g/R}{\Omega^2})^2) + \mathcal{O}(\theta^2) \tag{2.2.40}$$

  so the (circular) frequency of small vibrations is $\Omega \sin\theta_0$. For $\Omega < \sqrt{g/R}$ an expansion about $\theta = 0$ yields

  $$\ddot\theta = -\theta(\frac{g}{R} - \Omega^2) + \mathcal{O}(\theta^2) \tag{2.2.41}$$

  so the (circular) frequency is $\sqrt{g/R - \Omega^2}$. For $\Omega = \sqrt{g/R}$, the linear term in the Taylor series vanishes – the small vibration is not harmonic.
  This discussion of the behavior near the minima was intentionally done only in terms of forces, there is no need to invoke the effective potential at all. However, if the effective potential is known, the frequency of small vibrations is related to the curvature of that potential near the minima – we can think of this as approximating the potential near one of its minima with a harmonic oscillator, c.f. Fig. 11. One easily spots the qualitative change from one to two stable minima at some given value of $\frac{\Omega^2}{g/R}$ (which the analytical calculation reveals to be precisely 1). Such a behavior is called a bifurcation (of minima).

2.3 Variational principles and the Euler Lagrange equations

2.3.1 D'Alembert's principle as a variational principle

We begin with the observation that the constraint forces, if time independent, carry out no work. This can be verified by going back to Eq. (2.1.4) and looking at an individual particle i

$$\dot{\boldsymbol{p}}_i - \boldsymbol{F}_i - \sum_{I=1}^{k} \lambda^I(t)\boldsymbol{\nabla}_{\boldsymbol{r}_i} f^I(\boldsymbol{x}, t) = 0 \tag{2.3.1}$$

$$f^I(\boldsymbol{x}, t) = 0 \quad I = 1, \ldots, k < 3n \tag{2.3.2}$$

This is in a form that allows us to check energy conservation just as we have done earlier in Sec. 1.6.2 with the external forces $\boldsymbol{K}_i$ replaced by the constraint forces $\boldsymbol{C}_i = \sum_{I=1}^{k} \lambda^I(t)\boldsymbol{\nabla}_{\boldsymbol{r}_i} f^I(\boldsymbol{x}, t)$:

$$\dot{\boldsymbol{p}}_i \cdot \boldsymbol{p}_i/m = \frac{d}{dt}\Big(\underbrace{\frac{1}{2m_i}\boldsymbol{p}_i^2}_{=T_i}\Big) = -\frac{1}{m_i}\boldsymbol{p}_i \cdot \boldsymbol{\nabla}_{\boldsymbol{r}_i} \sum_{\substack{k=1 \\ k\neq i}}^{n} U_{ki}(\boldsymbol{r}_{ki}) + \frac{1}{m_i}\boldsymbol{p}_i \cdot \sum_{I=1}^{k} \lambda^I(t)\boldsymbol{\nabla}_{\boldsymbol{r}_i} f^I(\boldsymbol{x}, t) \tag{2.3.3}$$

Summing this over i we recover the time derivatives of total kinetic and potential energies being balanced by the work done by the constraint forces

$$\frac{d}{dt}(T+U)_{\text{total}} = \sum_{I=1}^{k} \lambda^I(t) \sum_i \dot{\boldsymbol{r}}_i \cdot \boldsymbol{\nabla}_{\boldsymbol{r}_i} f^I(\boldsymbol{x}, t) \tag{2.3.4}$$

Now note that

$$\frac{d}{dt} f^I(\boldsymbol{x}, t) = \sum_i \dot{\boldsymbol{r}}_i \cdot \boldsymbol{\nabla}_{\boldsymbol{r}_i} f^I(\boldsymbol{x}, t) + \frac{\partial}{\partial t} f^I(\boldsymbol{x}(t), t) \tag{2.3.5}$$

so that we may write

$$\frac{d}{dt}(T+U)_{\text{total}} = \sum_{I=1}^{k} \lambda^I(t) \left(\frac{d}{dt} - \frac{\partial}{\partial t} \right) f^I(\boldsymbol{x}(t), t) \tag{2.3.6}$$

Now imagine that the particle trajectories remain on the sub-manifold for all times t:

$$f^I(\boldsymbol{x}(t), t) = 0 \forall t \Rightarrow \frac{d}{dt} f^I(\boldsymbol{x}(t), t) = 0 \tag{2.3.7}$$

so that

$$\frac{d}{dt}(T+U)_{\text{total}} = -\sum_{I=1}^{k} \lambda^I(t) \frac{\partial}{\partial t} f^I(\boldsymbol{x}(t), t) \tag{2.3.8}$$

and we conclude that

> **If the constraints do not explicitly depend on time, no work is done by the constraint forces.**

Note that this makes strong use of the particle trajectories being subject to the constraints at all times as it relies on Eq. (2.3.7). This can in fact be turned around to state that virtual displacements $\delta \boldsymbol{x}^\alpha$ are those "small variations" of the physical system that are compatible with the condition that the constraints do no work, or only do work through explicit time dependence of the constraints. The system satisfies an extremality condition: certain small changes do not violate a certain condition, the system in an extremum of a function of some sort.

This is very similar to Fermat's principle: in an arbitrary system of mirrors and refracting glasses a light ray always chooses a path that is extremal (shortest or longest) between its source and the point where it is detected.

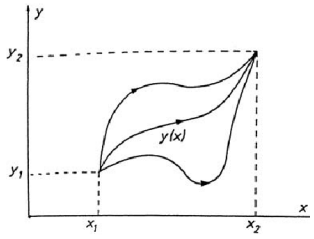
2.3.2 Elements of variational calculus

We will now see that the Lagrange equations can be viewed as the extremal conditions of a variational principle known as Hamilton's variational principle. To this end we need a few notions of variational calculus. What we are looking for is the extremum of some mathematical entity under a change from one trajectory of our system $\boldsymbol{x}_1(t)$ to another $x_2(t)$. Instead of talking about a space of coordinates, we talk about the space of trajectories on which we want to build some sort of "potential" function and look for extrema. To do so, we need to be able to do some sort of stability analysis and take derivatives in this space as well.

To this end, we define the one-parameter family of local variations of a function on an interval into a vector space V (which you may think of as configuration space $\mathfrak{C}$) $\boldsymbol{f} : [t_1, t_2] \to V$ which we require to be C^2

$$\boldsymbol{f}_s(t) = \boldsymbol{f}(t) + s\boldsymbol{\eta}(t) \tag{2.3.9}$$

where $\boldsymbol{\eta} : [t_1, t_2] \to V$ is C^2 and vanishes at the endpoints $\boldsymbol{\eta}(t_1) = \boldsymbol{\eta}(t_2) = \mathbf{0}$.



Fix graphics

Note that $\boldsymbol{f}_0(t) = \boldsymbol{f}(t)$ and that the derivatives with respect to s are well defined.

Imagine now an integral of the form

$$I[f] := \int_{t_1}^{t_2} dt' H[\boldsymbol{f}(t'), \dot{\boldsymbol{f}}(t'), t'] \tag{2.3.10}$$

for some function $H : V \times V \times [t_1, t_2] \to \mathbb{R}$: This integral will depend on f as a function. The only *explicit* t depdendence is through the endpoints t_i. We will call I a *functional* of $\boldsymbol{f}$ and start to look for stationary points of I under arbitrary one-parameter families of local variations (of the type (2.3.9)), i.e. we want to find the f for which

$$0 \overset{!}{=} \frac{d}{ds}\bigg|_{s=0} I[f_s] = \int_{t_1}^{t_2} dt' \, \frac{d}{ds}\bigg|_{s=0} H[\boldsymbol{f}_s(t'), \dot{\boldsymbol{f}}_s(t'), t'] \tag{2.3.11}$$

The derivatives are evaluated by chain rule. Suppressing the f-dependence of H for compactness we find:

$$= \int_{t_1}^{t_2} dt' \left[\frac{\partial H}{\partial f^\alpha} \frac{df_s^\alpha}{ds} + \frac{\partial H}{\partial \dot{f}^\alpha} \frac{d\dot{f}_s^\alpha}{ds} \right]_{s=0} = \int_{t_1}^{t_2} dt' \left[\frac{\partial H}{\partial f^\alpha} \frac{df_s^\alpha}{ds} + \frac{\partial H}{\partial \dot{f}^\alpha} \frac{d^2 f_s^\alpha}{ds dt} \right]_{s=0} \tag{2.3.12}$$

where α is summed from 1 to $\dim(V)$. Note that the derivatives in s and t in the last term commute so that we may partially integrate that last term in t to obtain

$$= \int_{t_1}^{t_2} dt' \left[\frac{\partial H}{\partial f^\alpha} \frac{df_s^\alpha}{ds} + \frac{d}{dt}\left(\frac{\partial H}{\partial \dot{f}^\alpha} \frac{df_s^\alpha}{ds} \right) - \left(\frac{d}{dt} \frac{\partial H}{\partial \dot{f}^\alpha} \right) \frac{df_s^\alpha}{ds} \right]_{s=0} \tag{2.3.13}$$

Now we use that $\frac{df_s^\alpha}{ds} = \eta^\alpha$

$$= \int_{t_1}^{t_2} dt' \left[\frac{\partial H[f, \dot{f}, t]}{\partial f^\alpha} - \frac{d}{dt} \frac{\partial H[f, \dot{f}, t]}{\partial \dot{f}^\alpha} \right] \eta^\alpha(t) + \underbrace{\left[\frac{\partial H[f, \dot{f}, t]}{\partial \dot{f}^\alpha} \eta^\alpha(t) \right]_{t_1}^{t_2}}_{=0 \text{ since } \boldsymbol{\eta}(t_i) = 0} \tag{2.3.14}$$

The last step is crucial: Since the $\eta^\alpha(t)$ are arbitrary functions of time inside the integral –and moreover independently arbitrary for each α– this leads to independent equations for the integrand for each α, called Euler's equations for the functional $I[f]$

$$\frac{\partial H[f,\dot{f},t]}{\partial f^\alpha} - \frac{d}{dt}\frac{\partial H[f,\dot{f},t]}{\partial \dot{f}^\alpha} = 0 \qquad \alpha = 1,\ldots,\dim(V) \tag{2.3.15}$$

The solutions to Eqns. (2.3.15) extremize the value of the functional $I[f]$ of Eq. (2.3.10).

Example 2.1 – Shortest distance between two points (in flat space):

Consider a curve $\boldsymbol{r}(\alpha)$ in $\mathbb{R}^3$, parametrized by a real parameter α connecting the points $\boldsymbol{r}(0) = \boldsymbol{x}$ and $\boldsymbol{r}(1) = \boldsymbol{y}$. Let us begin by noting that the length of the curve between the two endpoints must be independent on the way we parametize it. It can be obtained by integrating the magnitude of the tangent vector $\frac{d\boldsymbol{r}}{d\alpha}$ along the curve:

$$l[\boldsymbol{r}] = \int_0^1 d\alpha \left|\frac{d\boldsymbol{r}}{d\alpha}\right| = \int_0^1 d\alpha \sqrt{\left(\frac{d\boldsymbol{r}}{d\alpha}\right)^2} \tag{2.3.16}$$

Note that this expression is reparametrization invariant and completely generic – in relativity you will encounter the notion of proper time that is defined as a relativistic generalization of this construction. We note that the integrand in Eq. (2.3.18) is a reparametrization invariant length element.

I will present this calculation in two ways, first by retracing the arguments of the derivation of Eq. (2.3.15) step by step and secondly by using Eq. (2.3.15) directly.

Now introduce a one parameter family of variations

$$\boldsymbol{r}_s(\alpha) = \boldsymbol{r}(\alpha) + s\boldsymbol{\eta}(\alpha) \qquad \boldsymbol{\eta} \text{ smooth, with} \qquad \boldsymbol{\eta}(0) = \boldsymbol{\eta}(1) = 0\ , \tag{2.3.17}$$

to distort the curve without changing the endpoints.

The extremality condition for l then is

$$\begin{aligned}
0 =& \frac{d}{ds}\Big|_{s=0} l[\boldsymbol{r}_s] = \frac{d}{ds}\Big|_{s=0} \int_0^1 d\alpha \sqrt{\left(\frac{d\boldsymbol{r}_s}{d\alpha}\right)^2} \\
=& \int_0^1 d\alpha \frac{1}{2}\frac{1}{\sqrt{\left(\frac{d\boldsymbol{r}}{d\alpha}\right)^2}} \frac{d}{ds}\Big|_{s=0} \left(\frac{d\boldsymbol{r}_s}{d\alpha}\right)^2 = \int_0^1 d\alpha \frac{1}{2}\frac{1}{\sqrt{\left(\frac{d\boldsymbol{r}}{d\alpha}\right)^2}} 2\frac{d\boldsymbol{r}_s}{d\alpha}\frac{d}{d\alpha}\frac{d}{ds}\Big|_{s=0}\boldsymbol{r}_s \\
=& \int_0^1 d\alpha \frac{\frac{d\boldsymbol{r}}{d\alpha}}{\left|\frac{d\boldsymbol{r}}{d\alpha}\right|}\cdot\frac{d\boldsymbol{\eta}}{d\alpha} = \int_0^1 d\alpha \left[\frac{d}{d\alpha}\left(\frac{\frac{d\boldsymbol{r}}{d\alpha}}{\left|\frac{d\boldsymbol{r}}{d\alpha}\right|}\cdot\boldsymbol{\eta}\right) - \frac{d}{d\alpha}\frac{\frac{d\boldsymbol{r}}{d\alpha}}{\left|\frac{d\boldsymbol{r}}{d\alpha}\right|}\right] = -\int_0^1 d\alpha\ \boldsymbol{\eta}\cdot\left[\frac{d}{d\alpha}\frac{\frac{d\boldsymbol{r}}{d\alpha}}{\left|\frac{d\boldsymbol{r}}{d\alpha}\right|}\right]
\end{aligned} \tag{2.3.18}$$

with $\boldsymbol{\eta}$ arbitrary inside the integration region so that the integrand itself vanishes, component by component:

$$\frac{d}{d\alpha}\frac{\frac{d\boldsymbol{r}}{d\alpha}}{\left|\frac{d\boldsymbol{r}}{d\alpha}\right|} = 0 \tag{2.3.19}$$

We have to apply Eq. (2.3.15) with the identifications $t \to \alpha$, $f^i \to r^i$, $\dot{f}^i \to \frac{dr^i}{d\alpha} =: r'^i$, and $H \to \sqrt{\left(\frac{d\boldsymbol{r}}{d\alpha}\right)^2} = \sqrt{\boldsymbol{r}'^2}$:

$$0 \overset{!}{=} \left(\frac{\partial}{\partial r^i} - \frac{d}{d\alpha}\frac{\partial}{\partial r'^i}\right)\sqrt{\boldsymbol{r}'^2} = -\frac{d}{d\alpha}\frac{r'^i}{|\boldsymbol{r}'|} \tag{2.3.20}$$

Now that we have the extremality condition, we need to solve it. Here it is enough to simply interpret it:

$\frac{d\boldsymbol{r}}{d\alpha}$ represents a tangent to the curve with a magnitude that *will* depend on the parametrization chosen for the curve. The nomalized vector $\frac{\frac{d\boldsymbol{r}}{d\alpha}}{\left|\frac{d\boldsymbol{r}}{d\alpha}\right|}$ represents the unit vector in the same direction. Its magnitude is always 1 irrespective of the parametrization chosen and thus represents an intrinsinc feature of the extremal curve: The equation tells us that the direction of the tangent curve, the unit tangent vector $\frac{\frac{d\boldsymbol{r}}{d\alpha}}{\left|\frac{d\boldsymbol{r}}{d\alpha}\right|}$ does not change along the path. This leaves us with a straight line path connecting the endpoints.

Example 2.2 – the brachistochrone:

A Brachistochrone curve (Greek: brachistos - the shortest, chronos - time), or curve of fastest descent, is the curve between two points that a particle must follow to move from point $\boldsymbol{a}$ to point $\boldsymbol{b}$ in the shortest possible time if the initial velocity is zero and the accelerating force is provided by a constant field of gravity in the absence of friction.

To set this up we need a functional of the path $\boldsymbol{r}(t)$ that measure the time taken from endpoint to endpoint. To this end we need to combine the idea of path length with the idea of velocity. $dt = \frac{|\boldsymbol{v}|}{|\boldsymbol{v}|}dt$

Note that the numerator $|\boldsymbol{v}|dt = |\boldsymbol{r}'(\alpha)|d\alpha$ represents an invariant length element. (I have abbreviated $\boldsymbol{r}' := \frac{d\boldsymbol{r}}{d\alpha}$.) The $|\boldsymbol{v}|$ in the denominator we can trade for the z projection of $\boldsymbol{r}$ by energy conservation:

$$\frac{1}{2}m\boldsymbol{v}^2 = mg\hat{\boldsymbol{z}}\cdot\boldsymbol{r} \qquad \Rightarrow \qquad |\boldsymbol{v}| = \sqrt{2g\hat{\boldsymbol{z}}\cdot\boldsymbol{r}} \tag{2.3.21}$$

This is independent of parametrization as well. Then we can write our functional as

$$\Delta t = \frac{1}{\sqrt{2g}}\int_0^1 d\alpha\ \frac{\sqrt{\boldsymbol{r}'^2}}{\sqrt{\hat{\boldsymbol{z}}\cdot\boldsymbol{r}}} \tag{2.3.22}$$

Once again we introduce the a one parameter family of variations $\boldsymbol{r}_s(\alpha) = \boldsymbol{r}(\alpha) + s\boldsymbol{\eta}(\alpha)$, that leaves the endpoints fixed and derive an explicit form of the extremality condition directly from Eq. (2.3.15) (the constant prefactor $1/\sqrt{2g}$ can be cancelled at this point):

$$\begin{aligned} 0 \overset{!}{=}& \left(\frac{\partial}{\partial r^i} - \frac{d}{d\alpha}\frac{\partial}{\partial r'^i}\right)\frac{\sqrt{\boldsymbol{r}'^2}}{\sqrt{\hat{\boldsymbol{z}}\cdot\boldsymbol{r}}} = \sqrt{\boldsymbol{r}'^2}\frac{\partial}{\partial r^i}(\hat{\boldsymbol{z}}\cdot\boldsymbol{r})^{-\frac{1}{2}} - \frac{1}{\sqrt{\hat{\boldsymbol{z}}\cdot\boldsymbol{r}}}\frac{d}{d\alpha}\frac{\partial}{\partial r'^i}\sqrt{\boldsymbol{r}'^2} \\ =& -\frac{1}{2}\sqrt{\boldsymbol{r}'^2}(\hat{\boldsymbol{z}}\cdot\boldsymbol{r})^{-\frac{3}{2}}\delta^{i3} - (\hat{\boldsymbol{z}}\cdot\boldsymbol{r})^{-\frac{1}{2}}\frac{d}{d\alpha}\frac{\boldsymbol{r}'i}{|\boldsymbol{r}'|} \end{aligned} \tag{2.3.23}$$

or

$$\frac{d}{d\alpha}\frac{\boldsymbol{r}'i}{|\boldsymbol{r}'|}+\frac{1}{2}\frac{\sqrt{\boldsymbol{r}'^2}}{\hat{\boldsymbol{z}}\cdot\boldsymbol{r}}\hat{\boldsymbol{z}}=0 \tag{2.3.24}$$

Example 2.3 – the catenary:

The catenary is the shape assumed by hanging rope or chain of approximately uniform composition, suspended between two points in space and subject to uniform gravity.

The quantity to be extremised here is clearly the potential energy stored in the configuration. Assuming the object to be of uniform mass density ρ , the local contribution is $V_{\text{local}}(\boldsymbol{r}(\alpha))=\rho g\hat{\boldsymbol{z}}\cdot\boldsymbol{r}(\alpha)$

$$V_{\text{total}}[\boldsymbol{r}]=\int_{\boldsymbol{r}}d\alpha\sqrt{\boldsymbol{r}'^2}V_{\text{local}}(\boldsymbol{r}(\alpha))=\rho g\int d\alpha\hat{\boldsymbol{z}}\cdot\boldsymbol{r}(\alpha)\sqrt{\boldsymbol{r}'^2} \tag{2.3.25}$$

You will have noted that all three examples above end up producing a functional of the form

which is Fermat's principle. Interestingly also the geodesics in hyperbolic geometry fall into the same class. See [14] for a very elementary discussion.

Famous example: Brachistochrone

A Brachistochrone curve (Greek: brachistos - the shortest, chronos - time), or curve of fastest descent, is the curve between two points that is covered in the least time by a point-like body that starts at the first point with zero speed and is constrained to move along the curve to the second point, under the action of constant gravity and assuming no friction.

need to do this in 3d

First, we let a curve $y(x)$ that connects P and Q represent the curve. Assume $P=(a,y(a))$ and $Q=(b,y(b))$. We will restrict ourselves to curves that belong to $C^2[a,b]$. Given such a curve, the time it takes for the bead to go from P to Q is given by the functional (ds a length element, v the velocity)

$$I[y]:=\int_a^b\frac{ds}{v}=\int_a^b\frac{\sqrt{1+y'(x)}dx}{y(x)}$$

and allows us to find a differential equation for the solution $y(x)$.

Note that the associated Euler equations only assure us that the curve and time found this way is *extremal* – we still need to check if we have found a minimum or a maximum.

2.3.3 Hamilton's variational principle

Given the similarities of Lagrange's equations and the general form of Euler's equations for a functional allows us to state that in the absence of non-conservative forces the equations of motion of a constrained system can be obtained from a variational principle:

› **Concepts 2.2 – Hamilton's variational principle:**

Consider a mechanical system with f degrees of freedom, locally described by generalized coordinates $q^1, \ldots, q^f$, with kinetic and potential energies $T(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)$ and $U(\boldsymbol{q}, t)$, and Lagrangian

$$L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) = T(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) - U(\boldsymbol{q}, t) \ .$$

A physical orbit $\boldsymbol{q}(t)$ in the interval $[t_1, t_2]$ with boundary values $\boldsymbol{q}(t_1)$ and $\boldsymbol{q}(t_2)$ is an extremum of the *action integral*

$$S[\boldsymbol{q}] := \int_{t_1}^{t_2} dt \ L[\boldsymbol{q}, \dot{\boldsymbol{q}}, t] \ . \tag{2.3.26}$$

We use the term orbit of our physical system to generalize the notion of a trajectory since we include systems with more than one particle.

The physical orbit, i.e. the solution of the equations of motion for the specified boundary conditions, is singled out from all other possible orbits that the system might choose and that have the same boundary values by the requirement that the action integral take an extremal value.

For suitable choices of the boundary values at t_1 and t_2 this will often be a minimum, but that is not guaranteed: we might equally well encounter a maximum or a saddle point.

› **The Euler-Lagrange equations** associated with the action integral (2.3.26) through Hamilton's principle, are the set of equations

$$\frac{\delta L}{\delta q^\alpha} := \frac{\partial L}{\partial q^\alpha} - \frac{d}{dt}\frac{dL}{\partial \dot{q}^\alpha} = 0 \tag{2.3.27}$$

› **Further examples:**

- *An n-particle system without constraints* has the Lagrangian

$$L = T - U = \sum_i \frac{m_i \dot{\boldsymbol{r}}_i^2}{2} - U(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_n) \tag{2.3.28}$$

here $\boldsymbol{q} = (q^1, \ldots, q^{f=3n}) = (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_n)$ so that (no sum over α):

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^\alpha} - \frac{\partial L}{\partial q^\alpha} = m_{(\alpha)} \ddot{q}^\alpha + \frac{\partial U}{\partial q^\alpha} = 0 \tag{2.3.29}$$

($m_{(\alpha)}$ the mass associated with the index α) or

$$m_i \ddot{\boldsymbol{r}}_i + \boldsymbol{\nabla}_{\boldsymbol{r}_i} U(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_n) = 0 \tag{2.3.30}$$

- *A charged particle in an electric and magnetic field* satisfies the equation of motion

$$m\ddot{\boldsymbol{q}} = e\boldsymbol{E}(\boldsymbol{q}, t) + e\dot{\boldsymbol{q}}(t) \times \boldsymbol{B}(\boldsymbol{q}, t) \tag{2.3.31}$$

where we have identified $\boldsymbol{q} = \boldsymbol{r}$ and the expression on the right hand side is the Lorentz force. We have also denoted the charge of the particle e, referring to the most typical application, the electron in an electromagnetic field.

Expressing $\boldsymbol{E}$ and $\boldsymbol{B}$ via scalar and vector potential as

$$\boldsymbol{E}(\boldsymbol{q},t) = -\boldsymbol{\nabla}_{\boldsymbol{q}}\Phi(\boldsymbol{q},t) - \frac{1}{c}\frac{\partial}{\partial t}\boldsymbol{A}(\boldsymbol{q},t) \tag{2.3.32}$$

$$\boldsymbol{B}(\boldsymbol{q},t) = \boldsymbol{\nabla}_{\boldsymbol{q}} \times \boldsymbol{A}(\boldsymbol{q},t) \tag{2.3.33}$$

Eq. (2.3.31) can be obtained from the Lagrangian function

$$L(\boldsymbol{q},\dot{\boldsymbol{q}},t) := \frac{m}{2}\dot{\boldsymbol{q}}^2 - e\Phi(\boldsymbol{q},t) + e\dot{\boldsymbol{q}}\cdot\boldsymbol{A}(\boldsymbol{q},t) \tag{2.3.34}$$

Verify this claim!

From Wikipedia (*much more there*): Sir William Rowan Hamilton (4 August 1805 – 2 September 1865) was an Irish physicist, astronomer, and mathematician, who made important contributions to classical mechanics, optics, and algebra. His studies of mechanical and optical systems led him to discover new mathematical concepts and techniques. His greatest contribution is perhaps the reformulation of Newtonian mechanics, now called Hamiltonian mechanics. This work has proven central to the modern study of classical field theories such as electromagnetism, and to the development of quantum mechanics. In mathematics, he is perhaps best known as the inventor of quaternions.



From Wikipedia (*much more there*): Leonhard Euler (15 April 1707 – 18 September 1783) was a pioneering Swiss mathematician and physicist. He made important discoveries in fields as diverse as infinitesimal calculus and graph theory. He also introduced much of the modern mathematical terminology and notation, particularly for mathematical analysis, such as the notion of a mathematical function. He is also renowned for his work in mechanics, fluid dynamics, optics, and astronomy. Euler spent most of his adult life in St. Petersburg, Russia, and in Berlin, Prussia. He is considered to be the preeminent mathematician of the 18th century, and one of the greatest of all time.



2.3.4 Reconstructing the forces of constraint after the fact

The above discussion has allowed us to concentrate solely on the movement of the particles on the constraint surface, bypassing the constraint forces completely. The solutions to the Euler Lagrange equations $q^\alpha(t)$ with given initial conditions and the original choice of generalized coordinates gives us a handle on the full trajectories on the constraint surface in the original coordinates:

$$\boldsymbol{r}_i(t) = \boldsymbol{r}_i(\boldsymbol{q}(t)) \tag{2.3.35}$$

This needs examples!! The mathematical pendulum would be a good one.

From there it is easy to construct the *total* forces on the i-th particle

$$m_i\ddot{\boldsymbol{r}}_i(\boldsymbol{q}(t)) = F_i \tag{2.3.36}$$

and by projecting onto the directions of all $\boldsymbol{\nabla}_{r_i} f^I$, we can extract the constraint forces at any point at the trajectories.

Think of an engineer that needs to know the stresses on a rollercoaster!

2.3.5 Non-uniqueness of the Lagrangian

In all our discussion it is the equations of motion that determine the physics. Already these are not unique in the sense that any change of coordinate system will clearly affect their appearance. The same of course applies to the Lagrangian – it will change appearance as well if we change coordinate system. While that can usually be tracked by hand, we will collect how to systematically do this below.

There is additional freedom in the form of the Lagrangian that remains even if we keep our coordinate system fixed: We clearly may add terms to the Lagrangian that do not change the associated Euler-Lagrange equations. Such a change does not alter the physical system under consideration and the Lagrangians so obtained may be considered equivalent from a physics point of view.

2.3.5.1 Gauge transformations of the Lagrangian

We will require a little more and assume two Lagrangians L_1 and L_2 (expressed in the same set of coordinates) have the same variational derivatives, i.e.

$$\frac{\delta L_1}{\delta q^\alpha} \overset{!}{=} \frac{\delta L_2}{\delta q^\alpha} \tag{2.3.37}$$

irrespective of the question if the q^α satisfy the equations of motion $\frac{\delta L_i}{\delta q^\alpha} = 0$ or not.

To explore the implications of Eq. (2.3.39), we write the difference between the L_i as

$$L_2(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) - L_1(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) =: L_{21}(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) \tag{2.3.38}$$

and observe that (2.3.37) implies

$$0 \overset{!}{=} \frac{\delta L_{21}}{\delta q^\alpha} = \frac{d}{dt}\frac{\partial L_{21}}{\partial \dot{q}^\alpha} - \frac{\partial L_{21}}{\partial q^\alpha} = \frac{\partial^2 L_{21}}{\partial \dot{q}^\alpha \partial \dot{q}^\beta}\ddot{q}^\beta + \frac{\partial^2 L_{21}}{\partial \dot{q}^\alpha \partial q^\beta}\dot{q}^\beta + \frac{\partial^2 L_{21}}{\partial \dot{q}^\alpha \partial t} - \frac{\partial L_{21}}{\partial q^\alpha} \tag{2.3.39}$$

since $L_{21} = L_{21}(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)$ and does *not* depend on $\ddot{\boldsymbol{q}}$, the explicit factor $\ddot{q}^\beta$ in the first term of Eq. (2.3.39) is the only place where $\ddot{\boldsymbol{q}}$ appears at all. Since the equation must hold for any $\ddot{q}^\alpha$, $\dot{q}^\alpha$ and q^α, the coefficient of this term *must* vanish:

$$\frac{\partial^2 L_{21}}{\partial \dot{q}^\alpha \partial \dot{q}^\beta} = 0 \tag{2.3.40}$$

so that L_{21} can be at most linear in $\dot{\boldsymbol{q}}$:

$$L_{21} = \boldsymbol{A}(\boldsymbol{q}, t) \cdot \dot{\boldsymbol{q}} + B(\boldsymbol{q}, t) \tag{2.3.41}$$

where $\boldsymbol{A}(\boldsymbol{q}, t) \in \mathbb{R}^f$ and $B(\boldsymbol{q}, t)$ are arbitrary functions of $\boldsymbol{q}$ and t.

Inserting this back into Eq. (2.3.39) gives

$$\begin{aligned} 0 &\overset{!}{=} \underbrace{\frac{\partial^2(\boldsymbol{A}\cdot\dot{\boldsymbol{q}} + B)}{\partial \dot{q}^\alpha \partial q^\beta}\dot{q}^\beta}_{\frac{\partial A^\alpha}{\partial q^\beta}\dot{q}^\beta} + \underbrace{\frac{\partial^2(\boldsymbol{A}\cdot\dot{\boldsymbol{q}} + B)}{\partial \dot{q}^\alpha \partial t}}_{\frac{\partial A^\alpha}{\partial t}} - \underbrace{\frac{\partial(\boldsymbol{A}\cdot\dot{\boldsymbol{q}} + B)}{\partial q^\alpha}}_{\frac{\partial A^\beta}{\partial q^\alpha}\dot{q}^\beta - \frac{\partial B}{\partial t}} \\ &= \left(\frac{\partial A^\alpha}{\partial q^\beta} - \frac{\partial A^\beta}{\partial q^\alpha}\right)\dot{q}^\beta + \left(\frac{\partial A^\alpha}{\partial t} - \frac{\partial B}{\partial q^\alpha}\right) \end{aligned} \tag{2.3.42}$$

which must hold for all values of $\dot{\boldsymbol{q}}$. Since now the explicit factor of $\dot{\boldsymbol{q}}$ in Eq. (2.3.42) is the only place were $\dot{\boldsymbol{q}}$ appears, we conclude that the two terms in brackets must vanish separately:

$$\frac{\partial A^\alpha}{\partial q^\beta} - \frac{\partial A^\beta}{\partial q^\alpha} = 0 \qquad \text{and} \qquad \frac{\partial A^\alpha}{\partial t} - \frac{\partial B}{\partial q^\alpha} = 0 \; . \tag{2.3.43}$$

This is nothing but an integrability condition in $(\boldsymbol{q}, t)$-space, that allows us to write all of the A^α and B in terms of a common "potential" $M(\boldsymbol{q}, t)$:

$$A^\alpha = \frac{\partial M}{\partial q^\alpha} \qquad \text{and} \qquad B = \frac{\partial M}{\partial t} \tag{2.3.44}$$

Eq. (2.3.43) then simply states that the partial derivatives commute: In terms of M Eqns. (2.3.43) state that

$$\frac{\partial^2 M}{\partial q^\alpha \partial q^\beta} = \frac{\partial^2 M}{\partial q^\beta \partial q^\alpha} \qquad \text{and} \qquad \frac{\partial^2 M}{\partial q^\alpha \partial t} = \frac{\partial^2 M}{\partial t \partial q^\alpha} \; . \tag{2.3.45}$$

As a result $L_{21}(\boldsymbol{q}, t)$ is necessarily of the form

$$L_{21}(\boldsymbol{q}, t) = \frac{\partial M(\boldsymbol{q}, t)}{\partial q^\alpha} \dot{q}^\alpha + \frac{\partial M(\boldsymbol{q}, t)}{\partial t} = \frac{d}{dt} M(\boldsymbol{q}, t) \tag{2.3.46}$$

> **Concepts 2.3 – gauge transformations of the Lagrangian:**
> If two Lagrangians L_1 and L_2 in a given set of coordinates differ only by a total time derivative of a function $M(\boldsymbol{q}, t)$ that itself only depends on $\boldsymbol{q}$ and t (but *not* on $\dot{\boldsymbol{q}}$), then they lead to the same equations of motion.

This can be alternatively understood with the help of Hamilton's principle: Defining

$$S_i[\boldsymbol{q}] := \int_{t_1}^{t_2} dt \; L_i(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) \tag{2.3.47}$$

Hamilton's principle treats the EOM as a boundary value problem instead of an initial value problem.

then

$$S_2[\boldsymbol{q}] - S_1[\boldsymbol{q}] = \int_{t_1}^{t_2} dt \; \frac{d}{dt} M(\boldsymbol{q}, t) = M(\boldsymbol{q}(t_2), t_2) - M(\boldsymbol{q}(t_1), t_1) \; . \tag{2.3.48}$$

Since the variations are taken to vanish at the endpoints, this does not change the equations of motion. This highlights the purpose of a crucial feature of how we have introduced our one-parameter families of variations of our trajectories: The procedure fixes $\boldsymbol{q}(t_1)$ and $\boldsymbol{q}(t_2)$ instead of $\boldsymbol{q}(t_1)$ and $\dot{\boldsymbol{q}}(t_1)$, the way theorem 1 does. However, in both cases it is a set of $2f$ data that fully determine a solution.

This also explains why $M(\boldsymbol{q}, t)$ does not depend on $\dot{\boldsymbol{q}}$: we can not fix both $\boldsymbol{q}(t_1)$ and $\boldsymbol{q}(t_2)$ and then require any additional constraint on the $\dot{\boldsymbol{q}}(t_i)$. Note that our variational machinery as defined through one parameter families $\boldsymbol{q}(t) + s\boldsymbol{\eta}(t)$ generally *will* have different $\dot{\boldsymbol{q}}$ at the endpoints in accordance with this necessity: while $\boldsymbol{\eta}(t_i) = 0$, in general $\dot{\boldsymbol{\eta}}(t_i) \neq 0$.

› **Example:**
The natural L for the harmonic osciallator is $L = T - U$, i.e.

$$L = \frac{1}{2}\left(\left(\frac{dx}{dt}\right)^2 - x^2\right) \tag{2.3.49}$$

The function

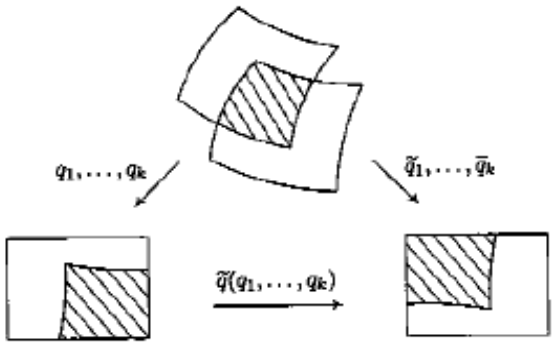
$$L' = \frac{1}{2}\left(\left(\frac{dx}{dt}\right)^2 - x^2\right) + x\frac{dx}{dt} \tag{2.3.50}$$

leads to the same equations of motion since $L' - L = \frac{d}{dt}\frac{x^2}{2}$

2.3.5.2 Admissible transformations of the generalized coordinates

Coordinate transformations between two sets of coordinates $\boldsymbol{q}$ and $\tilde{\boldsymbol{q}}$ that may suit our needs should at least be C^2 in the open sets U and $\tilde{U}$, where they are defined:

Fix graphics



We would clearly expect that a simple change of coordinates will not affect the physics encoded in the equations of motion:

Playing a little loose with time in our notation, we introduce a C^2 diffeomorphism of coordinates, which is defined on the image of the region $U \cap \tilde{U}$ in the configuration manifold where both coordinate systems are defined. Let me call this image, a subset of $\mathbb{R}^f$, U_1: $U_1 = q(U \cap \tilde{U}) \subset \mathbb{R}^f$. The change or coordinates takes us bijectively into $U_2 = \tilde{q}(U \cap \tilde{U}) \subset \mathbb{R}^f$.

$$g : U_1 \to U_2 \tag{2.3.51}$$

$$\boldsymbol{q} \mapsto \tilde{\boldsymbol{q}} = g(\boldsymbol{q}, t) \ , \tag{2.3.52}$$

which implies that g is locally invertible with C^2 inverse $g^{-1} : \tilde{\boldsymbol{q}} \mapsto \boldsymbol{q} = g^{-1}(\tilde{\boldsymbol{q}}, t)$ and

$$\det\left(\frac{\partial g^{-1\,i}(\tilde{\boldsymbol{q}}, t)}{\partial \tilde{q}^j}\right) \neq 0 \ . \tag{2.3.53}$$

Now we are equipped with the tools to consider the transformation induced for the Lagrangian. This can be conveniently read off from the following commuting diagram:

$$\begin{array}{ccc} \mathbb{R} & \xrightarrow{\quad \mathrm{id} \quad} & \mathbb{R} \\ L \uparrow & & \uparrow L' \\ \mathbb{R}^f \supset U_1 & \xrightarrow[g]{} & U_2 \subset \mathbb{R}^f \end{array} \qquad L' := \mathrm{id} \circ L \circ g^{-1} = L \circ g^{-1} \tag{2.3.54}$$

› **Remark 2.3 – commutative diagrams:**

This type of diagram is called a commutative diagram; you may traverse it any possible way along the edges and obtain the same result no matter what route you take to arrive at your destination.

This is *not* a mathematical torture device! Instead it is a rather useful tool to enlist a human's sense for the visual to reconstruct often rather complicated formulae, in this case how reconstruct the unkown L' from L and g.

We read off that

$$\begin{aligned} L'(\tilde{\boldsymbol{q}},\dot{\tilde{\boldsymbol{q}}},t) =&(L\circ g^{-1})(\tilde{\boldsymbol{q}},\dot{\tilde{\boldsymbol{q}}},t) = L(\boldsymbol{g}^{-1}(\tilde{\boldsymbol{q}},t),\frac{\partial \boldsymbol{g}^{-1}(\tilde{\boldsymbol{q}},t)}{\partial\tilde{q}^\alpha}\dot{\tilde{q}}^\alpha+\frac{\partial \boldsymbol{g}^{-1}(\tilde{\boldsymbol{q}},t)}{\partial t},t)\\ =&L(\boldsymbol{q}(\tilde{\boldsymbol{q}},t),\frac{\partial \boldsymbol{q}(\tilde{\boldsymbol{q}},t)}{\partial\tilde{q}^\alpha}\dot{\tilde{q}}^\alpha+\frac{\partial \boldsymbol{q}(\tilde{\boldsymbol{q}},t)}{\partial t},t) \end{aligned} \tag{2.3.55}$$

This should hopefully lead to the same physics, encoded in "transformed" equations of motion. Let's see:

$$\frac{\delta L'}{\delta\tilde{\boldsymbol{q}}^\alpha}=\frac{\partial L'}{\partial\tilde{q}^\alpha}-\frac{d}{dt}\frac{dL'}{\partial\dot{\tilde{q}}^\alpha} \tag{2.3.56}$$

Now we evalutate the two terms separately. The second term is easy since the $\dot{\tilde{\boldsymbol{q}}}$-dependence resides in the second slot alone:

$$\begin{aligned} \frac{d}{dt}\frac{dL'}{\partial\dot{\tilde{q}}^\alpha}=\frac{d}{dt}\left(\frac{dL}{\partial\dot{q}^\beta}\frac{\partial\dot{q}^\beta}{\partial\dot{\tilde{q}}^\alpha}\right)&\overset{(2.3.58)}{=}\frac{d}{dt}\left(\frac{dL}{\partial\dot{q}^\beta}\frac{\partial q^\beta}{\partial\tilde{q}^\alpha}\right)=\left(\frac{d}{dt}\frac{dL}{\partial\dot{q}^\beta}\right)\frac{\partial q^\beta}{\partial\tilde{q}^\alpha}+\frac{dL}{\partial\dot{q}^\beta}\frac{d}{dt}\frac{\partial q^\beta}{\partial\tilde{q}^\alpha}\\ &\overset{(2.2.21)}{=}\left(\frac{d}{dt}\frac{dL}{\partial\dot{q}^\beta}\right)\frac{\partial q^\beta}{\partial\tilde{q}^\alpha}+\frac{dL}{\partial\dot{q}^\beta}\frac{\partial\dot{q}^\beta}{\partial\tilde{q}^\alpha} \end{aligned} \tag{2.3.57}$$

where we have used

$$\frac{\partial \boldsymbol{q}(\tilde{\boldsymbol{q}},t)}{\partial\tilde{q}^\alpha}\dot{\tilde{q}}^\alpha+\frac{\partial \boldsymbol{q}(\tilde{\boldsymbol{q}},t)}{\partial t}\quad\Rightarrow\frac{\partial\dot{q}^\beta}{\partial\dot{\tilde{q}}^\alpha}=\frac{\partial q^\beta}{\partial\tilde{q}^\alpha} \tag{2.3.58}$$

The Last missing piece is

$$\frac{\partial L'}{\partial\tilde{q}^\alpha}=\frac{\partial L}{\partial q^\beta}\frac{\partial q^\beta}{\partial\tilde{q}^\alpha}+\frac{\partial L}{\partial\dot{q}^\beta}\frac{\partial\dot{q}^\beta}{\partial\tilde{q}^\alpha} \tag{2.3.59}$$

Adding (2.3.57) and (2.3.59) cancels the $\frac{\partial L}{\partial\dot{q}^\beta}\frac{\partial\dot{q}^\beta}{\partial\tilde{q}^\alpha}$ contributions and we are left with

$$\frac{\delta L'}{\delta\tilde{\boldsymbol{q}}^\alpha}=\frac{\delta L}{\delta\boldsymbol{q}^\beta}\frac{\partial q^\beta}{\partial\tilde{q}^\alpha}\ . \tag{2.3.60}$$

We read off:

› Since the matrix $\frac{\partial q^\beta}{\partial\tilde{q}^\alpha}$ is inertible (due to Eq. (2.3.53))

$$\frac{\delta L'}{\delta\tilde{\boldsymbol{q}}^\alpha}=0\Leftrightarrow\frac{\delta L}{\delta\boldsymbol{q}^\beta}$$

and the solutions to the equations of motion in found in one coordinate system are guaranteed to be solutions also in the other.

› The transformation behavior of the equations of motion is directly given by the Jacobian of the coordinate transformation: We say that the equations transform locally covariantly (i.e. locally like the basis vectors of the coordinate systems) under the change of coordinates.

3 Applications

3.1 Kepler's problem

The Kepler problem speaks of the gravitational interaction of two point particles of mass m_1 and m_2 located at positions $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ serving as a crude model for the sun–earth system and its celestial mechanics. The gravitational potential is a central potential, given as

$$U(\boldsymbol{r}_{12}) = -\frac{Gm_1m_2}{|\boldsymbol{r}_{12}|} \qquad \text{where in keeping with Sec. 1.6} \qquad \boldsymbol{r}_{12} := \boldsymbol{r}_1 - \boldsymbol{r}_2 \tag{3.1.1}$$

The system has $f = 3 \cdot 2$ degrees of freedom, there are no constraints to restrict the motion of the system, although, once the initial conditions are given, the conservation laws will restrict all subsequent motion to be compatible with them. This, we will see, will lead to strong simplifications of the problem.

Since there are no constraints, they do not provide any hint for the choice of a "suitable" coordinate system, but the system has conservation laws as was demonstrated in detail in Sec. 1.6:

- Conservation of total energy $\dot{E}_{\text{total}} = 0$ with $E_{\text{total}} = T_{\text{total}} + U_{\text{total}}$.
- Conservation of total (or Center of Mass (CM) momentum) $\dot{\boldsymbol{p}}_{\text{cm}} = 0$
- Conservation of total angular momentum $\dot{\boldsymbol{l}}_{\text{total}} = 0$

With the exception of energy all other conserved quantitities are related *directly* to acceleration of particles. Hence we expect both $\dot{\boldsymbol{p}}_{\text{cm}} = 0$ and $\dot{\boldsymbol{l}}_{\text{total}} = 0$ to appear in the EsOM rather directly: it turns out that they can be made explicit by a proper choice of coordinates.

To be able to easily implement such a choice, we utilize the Lagrangian formulation: Even in the absence of constraints, the equations of motion in *any* set of generalized coordinates (motivated by constraints or not) follow from the Lagrangian simply by evaluating

$$\frac{d}{dt}\frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)}{\partial \dot{q}^\alpha} - \frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)}{\partial q^\alpha} = 0 \tag{3.1.2}$$

where non conservative forces have been assumed to vanish.

Decoupling the system in CM/relative coordinates: $\dot{\boldsymbol{p}}_{\text{cm}} = 0$ can be made explicit by choseing CM and relative coordinates to parametrize T and U in the Lagrangian. This has the side effect of decoupling the CM motion from the EsOM of the remaining coordinates.

Recalling the definitions from Sec. 1.6.1

$$\boldsymbol{r}_{\text{cm}} := \frac{m_1\boldsymbol{r}_1 + m_2\boldsymbol{r}_2}{M}; \qquad \boldsymbol{r} := \boldsymbol{r}_1 - \boldsymbol{r}_2; \qquad M := m_1 + m_2; \mu := \frac{m_1m_2}{M} \tag{3.1.3}$$

one finds

$$T_{\text{total}} = \frac{m_1}{2}\dot{\boldsymbol{r}}_1^2 + \frac{m_2}{2}\dot{\boldsymbol{r}}_2^2 = \frac{M}{2}\dot{\boldsymbol{r}}_{\text{cm}}^2 + \frac{\mu}{2}\dot{\boldsymbol{r}}^2 \tag{3.1.4}$$

while the potential is expressed in terms of $\boldsymbol{r}$ already

$$U_{\text{total}}(\boldsymbol{r}_{12}) = U(\boldsymbol{r}) = -\frac{Gm_1m_2}{|\boldsymbol{r}|} = -\frac{GM\mu}{|\boldsymbol{r}|}\ , \tag{3.1.5}$$

so that

$$L = \frac{M}{2}\dot{\boldsymbol{r}}_{\text{cm}}^2 + \frac{\mu}{2}\dot{\boldsymbol{r}}^2 + \frac{GM\mu}{|\boldsymbol{r}|} \tag{3.1.6}$$

Note that we have changed variables for configuration space according to

$$\begin{pmatrix}\boldsymbol{r}_1\\ \boldsymbol{r}_2\end{pmatrix} \mapsto \begin{pmatrix}\boldsymbol{r}_{\text{cm}}\\ \boldsymbol{r}\end{pmatrix} =: \boldsymbol{q} \tag{3.1.7}$$

and the count of degrees of freedom remains identical.

Unlike $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ the new coordinates $\boldsymbol{r}_{\text{cm}}$ and $\boldsymbol{r}$ do not point at any physical particle. They discribe an equivalent pair of (independent) single particle systems with Eq. (3.1.7) providing the map between the two.

The new coordinates are special in the sense that their EsOM completely decouple:

$$0 = \frac{d}{dt}\frac{\partial L}{\partial \dot{r}^i_{\text{cm}}} - \frac{\partial L}{\partial r^i_{\text{cm}}} \qquad \text{independent of } \boldsymbol{r} \text{ for all components } i \tag{3.1.8}$$

$$0 = \frac{d}{dt}\frac{\partial L}{\partial \dot{r}^i} - \frac{\partial L}{\partial r^i} \qquad \text{independent of } \boldsymbol{r}_{\text{cm}} \text{ for all components } i \tag{3.1.9}$$

This is a simple consequence of the fact that the Lagrangian in the new coordinates splits into independent terms

$$L(\boldsymbol{q},\dot{\boldsymbol{q}}) = L(\boldsymbol{r}_{\text{cm}},\dot{\boldsymbol{r}}_{\text{cm}}) + L(\boldsymbol{r},\dot{\boldsymbol{r}}) \quad \text{where} \quad L(\boldsymbol{r}_{\text{cm}},\dot{\boldsymbol{r}}_{\text{cm}}) := \frac{M}{2}\dot{\boldsymbol{r}}_{\text{cm}}^2; \quad L(\boldsymbol{r},\dot{\boldsymbol{r}}) := \frac{\mu}{2}\dot{\boldsymbol{r}}^2 + \frac{GM\mu}{|\boldsymbol{r}|} \tag{3.1.10}$$

Center of mass and relative motion become completely independent and can be studied separately. This split has immediate consequences for the conservation laws of the system that follow without any further calculation:

- CM motion is subject to momentum conservation $\dot{\boldsymbol{p}}_{\text{cm}} = 0$. On the other hand, relative momentum $\boldsymbol{p} := \mu\dot{\boldsymbol{r}}$ is *not* conserved: the gravitational potential acts like an *external* potential on the fictitious particle of mass μ and provides a net external force!
- $\boldsymbol{l}_{\text{cm}} := M\boldsymbol{r}_{\text{cm}} \times \dot{\boldsymbol{r}}_{\text{cm}}$ and $\boldsymbol{l} := \mu\boldsymbol{r} \times \dot{\boldsymbol{r}}$ must be separately conserved. (CM motion is subject to no potential which certainly fits the bill of being radially symmetric, while the potential for relative motion exhibits its radial symmetry explicitly.)

  This does not imply that the number of independent conservation laws has gone up: $\dot{\boldsymbol{l}}_{\text{cm}} = 0$ is in fact a direct consequence of $\dot{\boldsymbol{p}}_{\text{cm}} = 0$ as verified in Eq. (3.1.15) below.
- The arguments leading up the conservation of total energy can be applied to CM motion and relative motion separately and lead to conservation of both $E_{\text{cm}} := \frac{\boldsymbol{p}_{\text{cm}}^2}{2M}$ and $E := \frac{\mu}{2}\dot{\boldsymbol{r}}^2 - \frac{GM\mu}{|\boldsymbol{r}|}$.

CM motion and conservation of total momentum: The EsOM for the CM coordinates are particularly simple, since $\frac{\partial L}{\partial r^i_{\text{cm}}} = 0$ for all $i = 1,2,3$, i.e. all components of $\boldsymbol{r}_{\text{cm}}$, we find

$$0 = \frac{d}{dt}\frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{\partial \dot{r}^i_{\text{cm}}} = \frac{d}{dt}M\dot{r}^i_{\text{cm}} = \frac{d}{dt}p^i_{\text{cm}}, \forall i = 1,2,3\ . \tag{3.1.11}$$

This is nothing but conservation of center of mass or total momentum of the system. Note that it was the choice of coordinates that made this explicit, $\boldsymbol{r}_{\text{cm}}$ is called a cyclical coordinate:

› **Concepts 3.1 – Cyclical coordinates:**
Generalized coordinates q^α for which $\frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{\partial q^\alpha} = 0$ are called cyclical. If present, they imply the existence of a conserved quantity, namely $\frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{\partial \dot{q}^\alpha}$, since the EOM for this coordinate simplifies to

$$\frac{d}{dt}\frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{\partial \dot{q}^\alpha} = 0 \tag{3.1.12}$$

Eq. (3.1.11) is immediately solved for the center of mass trajectory

$$\boldsymbol{r}_{\rm cm}(t) = \boldsymbol{r}_{\rm cm}(t_0) + \dot{\boldsymbol{r}}_{\rm cm}(t_0)(t-t_0) \tag{3.1.13}$$

in terms of its initial position and velocity $\boldsymbol{r}_{\rm cm}(t_0)$ and $\dot{\boldsymbol{r}}_{\rm cm}(t_0)$ at t_0.

This raises the question if angular momentum conservation can be made equally explicit? Before doing that, a quick check that the number of independent conservation laws has not changed in separating CM from relative motion is in order.

Cross check on separate conservation of $\boldsymbol{l}_{\rm cm}$ and $\boldsymbol{l}$: Note that total angular momentum can be written as a sum of CM and "relative" angular momentum:

$$\begin{aligned}\boldsymbol{l}_{\rm total} =& m_1\boldsymbol{r}_1\times\dot{\boldsymbol{r}}_1 + m_2\boldsymbol{r}_2\times\dot{\boldsymbol{r}}_2 = m_1(\boldsymbol{r}_{\rm cm}+\frac{m_2}{M}\boldsymbol{r})\times(\dot{\boldsymbol{r}}_{\rm cm}+\frac{m_2}{M}\dot{\boldsymbol{r}}) + m_2(\boldsymbol{r}_{\rm cm}-\frac{m_1}{M}\boldsymbol{r})\times(\dot{\boldsymbol{r}}_{\rm cm}-\frac{m_1}{M}\dot{\boldsymbol{r}})\\ =& M\boldsymbol{r}_{\rm cm}\times\dot{\boldsymbol{r}}_{\rm cm} + (1-1)\frac{m_1m_2}{M}(\boldsymbol{r}\times\dot{\boldsymbol{r}}_{\rm cm}+\boldsymbol{r}_{\rm cm}\times\dot{\boldsymbol{r}}) + \big(m_1\frac{m_2^2}{M^2}+m_2\frac{m_1^2}{M^2}\big)\boldsymbol{r}\times\dot{\boldsymbol{r}}\end{aligned}$$

where the cross terms in the products cancel between the two particle contributions so that we are left with

$$\boldsymbol{l}_{\rm total} = M\boldsymbol{r}_{\rm cm}\times\dot{\boldsymbol{r}}_{\rm cm} + \mu\boldsymbol{r}\times\dot{\boldsymbol{r}} = \boldsymbol{l}_{\rm cm} + \boldsymbol{l} \tag{3.1.14}$$

Note that also $\boldsymbol{l}_{\rm cm} := M\boldsymbol{r}_{\rm cm}\times\dot{\boldsymbol{r}}_{\rm cm}$ with pivot $\boldsymbol{r}_{\rm cm} = \boldsymbol{0}$, and $\boldsymbol{l} := \mu\boldsymbol{r}\times\dot{\boldsymbol{r}}$ with pivot $\boldsymbol{r} = \boldsymbol{0}$, do not describe the angular momentum of a "real" object in configuration space just like $\boldsymbol{r}_{\rm cm}$ and $\boldsymbol{r}$ do not describe real trajectories.

Note now that the result for CM motion in Eq. (3.1.13) directly implies that $\boldsymbol{l}_{\rm cm}$ is in fact time independent

$$\boldsymbol{l}_{\rm cm} = M(\boldsymbol{r}_{\rm cm}(t_0)+\dot{\boldsymbol{r}}_{\rm cm}(t_0)(t-t_0))\times\dot{\boldsymbol{r}}_{\rm cm}(t_0) = M\boldsymbol{r}_{\rm cm}(t_0)\times\dot{\boldsymbol{r}}_{\rm cm}(t_0) \tag{3.1.15}$$

and hence conserved. This, together with (3.1.14) implies that $\boldsymbol{l}$ is conserved on its own:

$$\dot{\boldsymbol{l}} = 0 \tag{3.1.16}$$

as argued on general grounds above.

Consequences of $\dot{\boldsymbol{l}} = 0$: $\dot{\boldsymbol{l}} = 0$ implies that all three componets of $\boldsymbol{l}$ are conserved. Alternatively, writing the relative angular momentum as a product of its direction $\hat{\boldsymbol{l}}$ and magntiude l,

$$\boldsymbol{l} = l\hat{\boldsymbol{l}} \tag{3.1.17}$$

emphasizes that both direction and magnitude are conserved separately. There is a special direction in the system and it turns out that motion is confined to a plane perpendicular to it that contains the pivot:

For a one particle system (as that describing the relative motion in our two particle system) with conserved angular momentum

$$\boldsymbol{l} = \boldsymbol{l}(t) = \mu \boldsymbol{r}(t) \times \dot{\boldsymbol{r}}(t) \stackrel{!}{=} \mu \boldsymbol{r}(t_0) \times \dot{\boldsymbol{r}}(t_0) \ , \tag{3.1.18}$$

The plane spanned by two vectors non-collinear vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ through $\boldsymbol{c}$ is the set $\{\boldsymbol{r} = \alpha\boldsymbol{a} + \beta\boldsymbol{b} + \boldsymbol{c} | \alpha, \beta \in \mathbb{R}\}$.

$\boldsymbol{r}(t)$ is constrained to the plane through the *origin* (the pivot) spanned by $\dot{\boldsymbol{r}}(t_0)$ and $\dot{\boldsymbol{r}}(t_0) \times \boldsymbol{l}$.

Thus, if one chooses a coordinate system that aligns $\hat{\boldsymbol{z}}$ with $\boldsymbol{l}$, any initial conditions with arbitray $\boldsymbol{r}(t_0)$ and $\dot{\boldsymbol{r}}(t_0)$ will *automatically* have $z(t_0) = 0$ and $\dot{z}(t_0) = \hat{\boldsymbol{z}} \cdot \dot{\boldsymbol{r}}(t_0) = 0$ *in this "aligned" coordinate system.* The argument given above states in addition that $z(t) = 0$ and $\dot{z}(t) = 0$ for *all* times.

To adapt to the situation we plan to align our z-axis with $\boldsymbol{l}$ and parametrize the directions perpendicular to that axis using a polar coordinate system, i.e. we choose a cylindrical orthonormal coordinate basis

$$\hat{\boldsymbol{z}} = (0,0,1)^t; \qquad \hat{\boldsymbol{r}}(\varphi) = (\cos\varphi, \sin\varphi, 0)^t; \qquad \text{and} \qquad \hat{\boldsymbol{\varphi}}(\varphi) = (-\sin\varphi, \cos\varphi, 0)^t; \tag{3.1.19}$$

so that

$$\boldsymbol{r} = r\hat{\boldsymbol{r}}(\varphi) + z\hat{\boldsymbol{z}} \tag{3.1.20}$$

From here one may directly calculate velocities to find

$$\dot{\boldsymbol{r}} = \dot{r}\hat{\boldsymbol{r}}(\varphi) + r\dot{\hat{\boldsymbol{r}}}(\varphi) + \dot{z}\hat{\boldsymbol{z}} = \dot{r}\hat{\boldsymbol{r}}(\varphi) + r\dot{\varphi}\frac{\partial}{\partial\varphi}\hat{\boldsymbol{r}}(\varphi) + \dot{z}\hat{\boldsymbol{z}} = \dot{r}\hat{\boldsymbol{r}}(\varphi) + r\dot{\varphi}\hat{\boldsymbol{\varphi}}(\varphi) + \dot{z}\hat{\boldsymbol{z}} \ , \tag{3.1.21}$$

so that

$$\dot{\boldsymbol{r}}^2 = (\dot{r}^2 + r^2\dot{\varphi}^2) + \dot{z}^2 \ . \tag{3.1.22}$$

The Lagrangian for the relative motion now reads

$$L = \frac{\mu}{2}\big((\dot{r}^2 + r^2\dot{\varphi}^2) + \dot{z}^2\big) + \frac{GM\mu}{\sqrt{r^2+z^2}} \tag{3.1.23}$$

and if we trust our argument for that $z(t) = 0$ and $\dot{z}(t) = 0$ for *all* times we may just drop these contributions and all that is left is a two-dimensional problem for r and φ. This is what is done in most textbooks. If one feels the need to be overly careful, one can check that this is consistent by looking at the EsOM that emerge before we eliminate z. They read

$$0 = \frac{d}{dt}\frac{\partial L}{\partial \dot{z}} - \frac{\partial L}{\partial z} = \frac{d}{dt}\mu\dot{z} - (-\tfrac{1}{2})\frac{GM\mu}{(r^2+z^2)^{3/2}}2z \quad \text{i.e.} \quad 0 = \mu\ddot{z} + GM\mu\frac{z}{(r^2+z^2)^{3/2}} \tag{3.1.24a}$$

$$0 = \frac{d}{dt}\frac{\partial L}{\partial \dot{r}} - \frac{\partial L}{\partial r} \quad \text{i.e.} \quad 0 = \mu\ddot{r} - \mu r\dot{\varphi}^2 + GM\mu\frac{r}{(r^2+z^2)^{3/2}} \tag{3.1.24b}$$

$$0 = \frac{d}{dt}\frac{\partial L}{\partial \dot{\varphi}} - \frac{\partial L}{\partial \varphi} \quad \text{i.e.} \quad 0 = \frac{d}{dt}\mu r^2\dot{\varphi} \tag{3.1.24c}$$

and note that they permit a solution with $z(t) = 0$ for all times, it corresponds to *initial conditions* where $z(t_0) = 0$ $\dot{z}(t_0) = 0$. For this solution the general expression for $\boldsymbol{l}$ reduces to

$$\boldsymbol{l} = \mu\boldsymbol{r} \times \dot{\boldsymbol{r}} = \mu\big(r^2\dot{\varphi}\hat{\boldsymbol{r}} \times \hat{\boldsymbol{\varphi}} + (r\dot{z} - z\dot{r})\hat{\boldsymbol{r}} \times \hat{\boldsymbol{z}} + zr\dot{\varphi}\hat{\boldsymbol{z}} \times \hat{\varphi}\big) = \mu r^2\dot{\varphi}\hat{\boldsymbol{z}} \tag{3.1.25}$$

with $\hat{\boldsymbol{l}} = \hat{\boldsymbol{z}}$ as reqired. Moreover one infers that the magnitude of the angular momentum l is given by $l = \mu r^2\dot{\varphi}$.

Eq. (3.1.24c) now identifies l as a cyclial coordinate and simply expresses angular momentum conservation and one may use it to eliminate $\dot{\varphi}$ from the equation for r at $z = 0$ to arrive at a one dimensional problem:

$$0 = \mu\ddot{r} - \frac{l^2}{\mu r^3} + \frac{GM\mu}{r^2} \tag{3.1.26}$$

Physically this equation describes one dimensional motion subject to an effective conservative force

$$F_{\text{eff}} := \frac{l^2}{\mu r^3} - \frac{GM\mu}{r^2} = -\frac{d}{dr}U_{\text{eff}}(r) \quad \text{with} \quad U_{\text{eff}}(r) := \frac{l^2}{2\mu r^2} + U(r) \tag{3.1.27}$$

> **Warning 3.1 – Restrictions from conservation laws vs constraints:**
> In the discussion of Kepler's problem many texts assert from the outset that angular momentum conservation restricts the relative motion to a plane. The discussion above clarifies that this is not an external constraint that is imposed on the system, instead, one solves the equations of motion and chooses some set of initial conditions. It is that set of initial conditions that determines all conserved quantities at the outset (such as angular momentum) and determines which plane becomes the plane of motion that Noether's theorem asserts to exist. Initial conditions $\boldsymbol{r}_0$ and $\boldsymbol{v}_0$ determine the magnitude and orientation of the conserved quantity, $\boldsymbol{l} = \boldsymbol{l}_0 = \boldsymbol{r}_0 \times (\mu\boldsymbol{v}_0)$. Relative motion is then restriced to a plane though the origin, being spanned by either $\boldsymbol{r}_0$ and $\boldsymbol{v}_0$ or equivalently by $\boldsymbol{v}_0$ and $\boldsymbol{v}_0 \times \boldsymbol{l} = \boldsymbol{v}_0^2(\mathbb{1} - \hat{\boldsymbol{v}}_0 \otimes \hat{\boldsymbol{v}}_0)\boldsymbol{r}_0$. The latter charcterises it as a plane perpendicular to $\boldsymbol{l}$.

What is left is to find a solution to the equation of radial motion, Eq. (3.1.26). Before we do this quantitatively, let us appeal to energy conservation and the notion of effective potentials to get a qualitative understanding of the behavior.

Energy conservation and effective potentials: The only conservation law we have not encountered directly in our previous discussion is the conservation of total energy. In fact, the split into CM and relative motion components also applies to the energy of the system

$$E_{\text{total}} = E_{\text{cm}} + E \quad \text{where} \quad E_{\text{cm}} := \frac{M}{2}\dot{\boldsymbol{r}}_{\text{cm}}^2; \quad E := \frac{\mu}{2}\dot{\boldsymbol{r}}^2 + U(|\boldsymbol{r}|) \tag{3.1.28}$$

As with CM angular momentum, convervation of E_{cm} follows directly from the center of mass principle via $E_{\text{cm}}(t) = \frac{M}{2}[\dot{\boldsymbol{r}}_{\text{cm}}(t_0)]^2$ so that conservation of total energy also implies conservation of energy for the subsystem of relative motion $\dot{E} = 0$.

In fact in the aligned coordinate system (3.1.19) at $z = 0$ with fixed l we have

$$E = \frac{\mu}{2}\dot{r}^2 + \frac{l^2}{2\mu r^2} + U(r) = \frac{\mu}{2}\dot{r}^2 + U_{\text{eff}}(r) \tag{3.1.29}$$

and one can infer allowed regions of motion for fixed energy E and angular momentum l in a plot of $U_{\text{eff}}(r)$ since kinetic energy and total energy must sum to E the allowed regions are those where $E > U_{\text{eff}}$ and the radial velocity $\dot{r}$ must become zero where $E = U_{\text{eff}}$.

The most striking feature of U_{eff} is its *angular momentum barrier*, the term $\frac{l^2}{2\mu r^2}$, which is always repulsive provided $l > 0$.

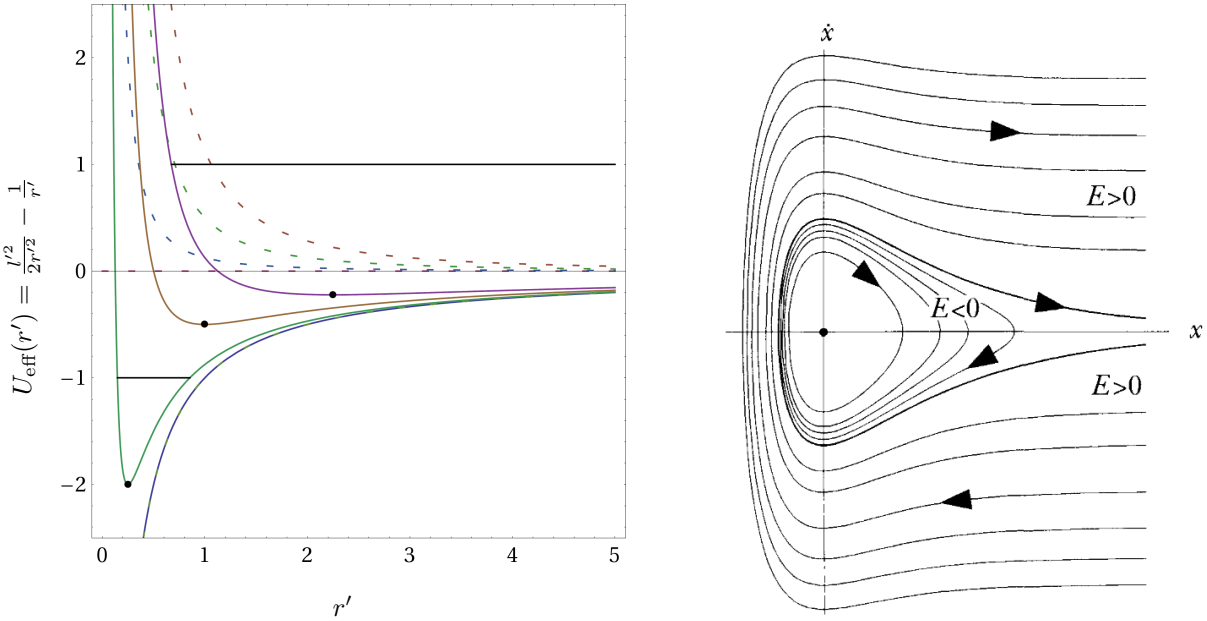


Fig. 12: ***Left:*** *effective potential of the Kepler problem (bold lines) against* $r' := \frac{r}{GM\mu}$ *for* $l' := \frac{l}{GM\mu^{3/2}} = 0, .5, 1, 1.5$ *and angular momentum barrier for the same values of* l' *(dashed). Bound states at* $E < 0$ *show two turning points at minimal and maximal radii, scattered states have trajectories* $E > 0$*, come in from* ∞ *to reach a point of closest approach and return to* ∞*. The black dots mark the extrema of* U_{eff} *for which the radii are not time dependent. These correspond to circular orbits.* ***Right:*** *Phase space trajectories for the Keper problem show closed orbits for* $E < 0$ *and open orbits for* $E > 0$*.*

3.1.1 Foucault's pendulum, or "how to prove quantiatively that the earth is rotating witout resorting to astronomy"

The restoring force, in the small-angle approximation to the oscillation, is given by

$$F_{g,x} = -m\omega^2 x \tag{3.1.30}$$

$$F_{g,y} = -m\omega^2 y. \tag{3.1.31}$$

Since a frame erected on the surface of the earth is not an inertial but a rotating frame, we have to deal with both Coriolis and centrifugal forces.

We recall from Eq. 1.5.8 that Newton's equations in a rotating frame A which shares the origin with an inertial frame B, read

$$m\ddot{\boldsymbol{x}}^A = (\boldsymbol{F}^B(t))^A - m(\Omega^a i t^a)^2 \boldsymbol{x}^A(t) - 2m(\Omega^a i t^a)\dot{\boldsymbol{x}}^A(t) \tag{3.1.32}$$

This is not quite what we need here, since the frame we erect on the surface of the earth is, in addition, offset from the center of the earth, but that we can absorb in the z coordinate of the frame A.

Which inertial frame you might ask? We have several types of rotational motion superimposed on any point of the surface of our earth. There is the rotation of the earth around its axis, with a frequency $\Omega = 1/\text{day} = \frac{1}{.864\cdot 10^5 \text{s}}$. There is the earth's rotation about the sun with a frequency of $\Omega' = 1/\text{year} \approx (.3155 \cdot 10^8 \text{s})^{-1}$, i.e. 3 orders of magnitude off and that of the solar system around the galactic center. The time for one

such revolution is called a Galactic year and estimated to be around 225-250 million (terrestrial) years, again a factor 10^{3+6}, i.e. 9 orders of magnitude further off. Any noninertial components of motion beyond that become very hard to identify indeed. That fact alone should provide a hint that they are not relevant to the task at hand. So: how do we decide on which level to stop? How do we rank the forces involved? Aside from the rotational frequencies, we need estimates of the the distances invloved (to get the mangitude of the centrifugal force involved and consider that for a bound orbit, this contribution might be balanced by a gravitational attraction) and the typical angular velocities $\dot{\boldsymbol{x}}^A$.

finish Foucault approx

We need to set up suitable coordinate systems to discuss this. In a purely academic problem, one would expect to simply set this up in spherical coordinates. Since we are talking about an experimental setup on earth, we are faced with coordinate conventions commonly used in this setting as well. Instead of the polar angle θ one typically uses a latitude angle, anchored at the equator. The two are related by $\theta = \frac{\pi}{2} - \varphi_{\text{lat}}$

The local coordinate system is given by

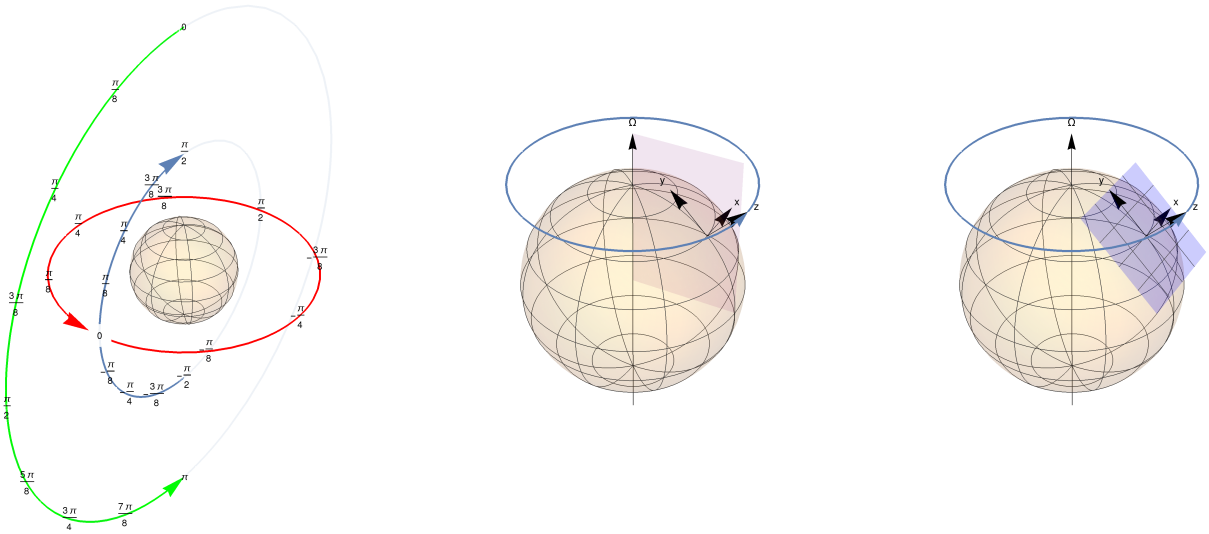


Fig. 13: *Relating the local coordinate system with standard spherical coordinates.*

Using Newton's laws of motion this leads to the system of equations

$$\frac{d^2x}{dt^2} = -\omega^2 x + 2\Omega \frac{dy}{dt} \sin(\varphi_{\text{lat}}) \tag{3.1.33}$$

$$\frac{d^2y}{dt^2} = -\omega^2 y - 2\Omega \frac{dx}{dt} \sin(\varphi_{\text{lat}})\,. \tag{3.1.34}$$

Or, in matrix form on $\mathbb{R}^2$:

$$\ddot{\boldsymbol{r}} = -\omega^2 \boldsymbol{r} - 2\Omega \sin(\varphi_{\text{lat}}) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \dot{\boldsymbol{r}} \tag{3.1.35}$$

Switching to complex coordinates $z = x + iy$, the equations read

$$\frac{d^2z}{dt^2} + i2\Omega \sin(\varphi_{\text{lat}}) \frac{dz}{dt} + \omega^2 z = 0\,. \tag{3.1.36}$$

We can compare the complex version of this to the damped harmonic oscillator and note that the equations look structurally identical with an imaginary constant $i2\Omega\sin(\varphi_{\text{lat}})$ replacing the damping constant γ. The general solution found earlier is thus easily adapted. Defining the shifted harmonic frequency

$$\tilde{\omega} := \sqrt{\omega^2 + (2\Omega\sin(\varphi_{\text{lat}}))^2} \in \mathbb{R} \tag{3.1.37}$$

we obtain

$$\begin{aligned} z(t) = e^{-i2\Omega\sin(\varphi_{\text{lat}})(t-t_0)} \Bigg[\left(\cos(\tilde{\omega}(t-t_0)) + \frac{\sin(\tilde{\omega}(t-t_0))}{\tilde{\omega}} i2\Omega\sin(\varphi_{\text{lat}}) \right) z(t_0) \\ + \frac{\sin(\tilde{\omega}(t-t_0))}{\tilde{\omega}} \dot{z}(t_0) \Bigg] \end{aligned} \tag{3.1.38}$$

and can immediately verify that this solves Eq. (3.1.36).

The overall prefactor $e^{-i2\Omega\sin(\varphi_{\text{lat}})(t-t_0)}$ describes a uniform rotation of the pattern of motion prescribed by the expression in the square brackets. The term porportional to $z(t_0)$ traces out a "rescaled circle", i.e. a circle where the axis perpendicular to $z(t_0)$ is rescaled by $2\Omega\sin(\varphi_{\text{lat}})/\tilde{\omega}$. The term proportional to the initial velocity superposes harmonic motion in the direction of $\dot{z}(t_0)$.

The resulting patterns become quite intricate unless we look at pathological cases such as the limit of $\Omega \to \infty$ (i.e. the limit where the rotation period of earth becomes shorter and shorter) while you keep ω fixed. If $\ddot{z}(t_0) = 0$, this leads to a stationary pendulum.

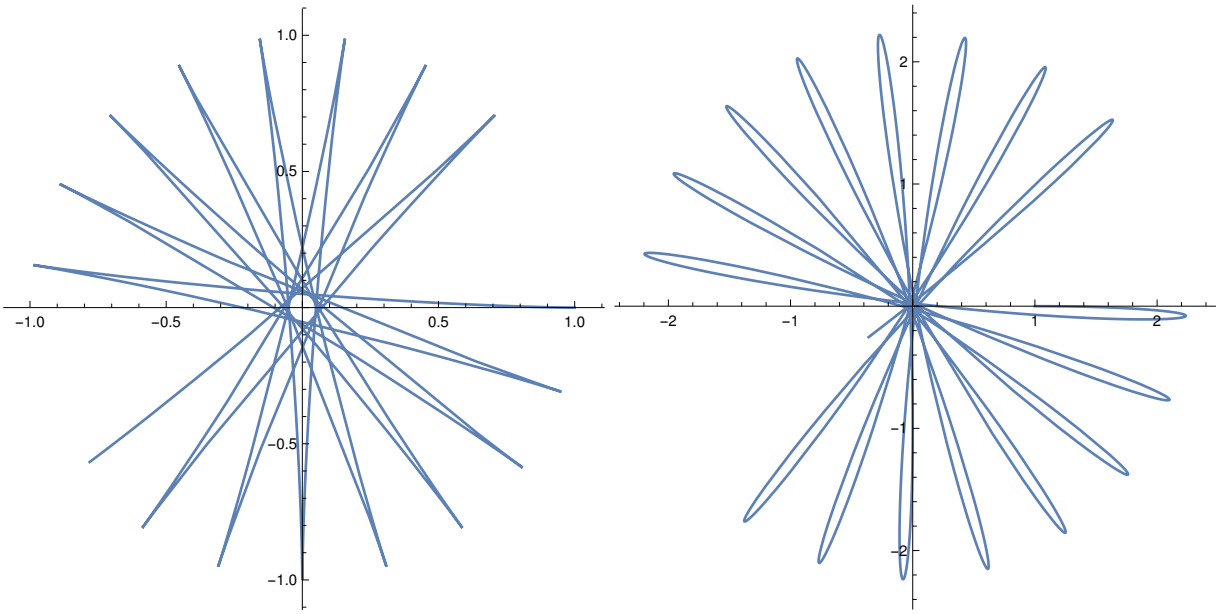


Fig. 14: *Foucault traces* ./Foucault.nb

The web is full of assertions that the behavior of the pendulum is geometric in nature and can be explained by parallel transport. This is indeed true for the overall phase $e^{-i2\Omega\sin(\varphi_{\text{lat}})(t-t_0)}$, but noes not apply to the $\frac{\sin(\tilde{\omega}(t-t_0))}{\tilde{\omega}} i2\Omega\sin(\varphi_{\text{lat}}) z(t_0)$ term in the above. Note, however, that for a pendulum on earth $\omega^2 = \frac{g}{l} \approx .98 \cdot 10^1 \frac{\text{m}}{\text{s}^2} \frac{1}{l}$, while $\Omega^2 = \text{day}^{-2} \approx (.864 \cdot 10^5\text{s})^{-2}$ ($\Omega'^2 = \text{year}^{-2} \approx (.3155 \cdot 10^8\text{s})^{-2}$) , so that $\frac{\Omega^2}{\omega^2} \ll 1$ and the correction is indeed tiny unless we imagine a gigantic pendulum ($l \gtrapprox 10^5\text{m}$).

Foucault-resources/BachelorThesisMortenIbMunk-Nielsen.pdf

Also look at Kristopher Tapp's "Differential Geometry of Curves and Surfaces" [15], sec 5.

3.2 Rigid bodies, spinning tops

› Michael Spivak in his "Physics for Mathematicians – Mechanics I" [16][5] has a strangely inspiring opening discussion on levers and the role rigidity of a balances arms play in their operation.

[5] I do not know of any followup publications that seem to be implied my the "Mechanics I" in the title.

4 The Hamiltonian description of classical mechanics

4.1 Towards a phase space description with generalized coordinates

Hamilton's description of a mechanical system is an alternative formulation of classical mechanics that replaces the Lagrangian as its central tool by what is known as the Hamiltonian of the system and replaces generalized velocities $\dot{\boldsymbol{q}}$ with as suitable set of generalzised momenta $\boldsymbol{p}$ (yet to be defined). The starting point to introduce these objects are conservation laws and an attempt to rewrite the Euler-Lagrange equations in a first order (phase space) form.

Observation 1 – a conserved quantity: Start from the Lagrangian of a system in generalized coordinates

$$L(\boldsymbol{q},\dot{\boldsymbol{q}},t) = T(\boldsymbol{q},\dot{\boldsymbol{q}},t) - U(\boldsymbol{q},t) \tag{4.1.1}$$

and consider the function

Summation convention on α!

$$\tilde{H}(\boldsymbol{q},\dot{\boldsymbol{q}},t) := \dot{q}^\alpha \frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{\partial \dot{q}^\alpha} - L(\boldsymbol{q},\dot{\boldsymbol{q}},t) \tag{4.1.2}$$

Its time derivative is easily calculated

cancel directly

$$\frac{d\tilde{H}(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{dt} = \ddot{q}^\alpha \frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{\partial \dot{q}^\alpha} + \dot{q}^\alpha \frac{d}{dt}\frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{\partial \dot{q}^\alpha} - \frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{\partial q^\alpha}\dot{q}^\alpha - \frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{\partial \dot{q}^\alpha}\ddot{q}^\alpha - \frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{\partial t} \tag{4.1.3}$$

zero on EOM

That is, on solutions of the EsOM

$$\frac{d\tilde{H}(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{dt} = \frac{d}{dt}\left(\dot{q}^\alpha \frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{\partial \dot{q}^\alpha} - L(\boldsymbol{q},\dot{\boldsymbol{q}},t)\right) = -\frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{\partial t}\ . \tag{4.1.4}$$

For *autonomous systems*, where both L and $\tilde{H}$ do not explicitly depend on time ($\frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{\partial t} = \frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial t} = 0$), this result is often referred to as the Beltrami identity

$$\tilde{H}(\boldsymbol{q},\dot{\boldsymbol{q}}) := \dot{q}^\alpha \frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha} - L(\boldsymbol{q},\dot{\boldsymbol{q}}) \overset{!}{=} \text{const. on solutions of the EsOM}\ . \tag{4.1.5}$$

$\tilde{H}(\boldsymbol{q},\dot{\boldsymbol{q}})$ is a *constant of motion*, i.e. it is conserved for solution of the equations of motion.

Observation 2 – it is the energy in certain cases: What is the interpretation of this conserved quantity? An example will provide a hint. Take a single particle in a central potential

$$L(\boldsymbol{r},\dot{\boldsymbol{r}}) = m\dot{\boldsymbol{r}}^2/2 - U(\boldsymbol{r}) = T(\boldsymbol{r},\dot{\boldsymbol{r}}) - U(\boldsymbol{r}) \quad \Rightarrow \quad \tilde{H}(\boldsymbol{r},\dot{\boldsymbol{r}}) = 2T - (T-U) = m\dot{\boldsymbol{r}}^2/2 + U(\boldsymbol{r}) \tag{4.1.6}$$

The conserved quantity in this particular case is the total energy of the system. The reason this occurs is, that

$$\dot{q}^\alpha \frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha} = 2T \tag{4.1.7}$$

in this particular case.

Observation 3 – first order EsOM in terms of q^α and p^α and H: To be able to write the EsOM in the form $\dot{q}^\alpha = \ldots$, $\dot{p}^\alpha = \ldots$ we attempt to eliminate $\dot{\boldsymbol{q}}$ in favor of $\boldsymbol{p}$, i.e. we attempt to write $\dot{\boldsymbol{q}}$ as a function of $\boldsymbol{q}, \boldsymbol{p}$, and t: $\dot{\boldsymbol{q}} = \dot{\boldsymbol{q}}(\boldsymbol{q}, \boldsymbol{p}, t)$. This is trivial in our example: We observe that

We leave the ~ off, now that we have expressed the function in terms of $\boldsymbol{q}$ and $\boldsymbol{p}$.

$$p^i = m\dot{r}^i = \frac{\partial L}{\partial \dot{r}^i} \tag{4.1.8}$$

and use this to read $\boldsymbol{r}$ as a function of $\boldsymbol{p}$ (it is independent of $\boldsymbol{r}$ in this case). Then $\tilde{H}$, interpreted as a function of $\boldsymbol{r}$ and $\boldsymbol{p}$, i.e. as

$$H(\boldsymbol{r}, \boldsymbol{p}) = \frac{\boldsymbol{p}^2}{2m} + U(\boldsymbol{r}) = T(\boldsymbol{r}, \boldsymbol{p}) + U(\boldsymbol{r}) \tag{4.1.9}$$

allows us to express the equations of motion in the form

$$\dot{r}^i = \frac{p^i}{m}; \qquad \dot{p}^i = -\nabla^i U(\boldsymbol{r}) \tag{4.1.10}$$

This is indeed just the first order formulation of Newton's equations alluded to in Sec. 1.7 when we introduced the phase space formulation.

We and observe that the right hand sides (in this particular case) can be interpreted as derivatives of H:

$$\dot{r}^i = \frac{\partial H}{\partial p^i}; \qquad \dot{p}^i = -\frac{\partial H}{\partial r^i} \tag{4.1.11}$$

Since this form of the equations appears to be particularly well adapted to the phase space picture, it might be profitable to explore if, and under which circumstances such a transformation can be achieved in the more general case in which constraints may be present.

› **Canonically conjugate momentum and cyclical coordinates:**

Taking our hint from Eq. (4.1.8) to define *canonically conjugate momentum* p^α for every generalized coordinate q^α via

$$p^\alpha := \frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)}{\partial \dot{q}^\alpha} \tag{4.1.12}$$

Note that the equations of motion

$$\frac{\delta L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)}{\delta q^\alpha} = \frac{\partial L}{\partial q^\alpha} - \frac{d}{dt}\frac{dL}{\partial \dot{q}^\alpha} \stackrel{!}{=} 0 \tag{4.1.13}$$

tell us that this momentum is conserved or an *integral of motion*, whenever $\frac{\partial L}{\partial q^\alpha} = 0$, i.e. if L does not depend on the corresponding coordinate. Such generalized coordinates are called cyclical coordinates.

At this stage we have set the stage by introducing

$$\tilde{H}(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) := \dot{q}^\alpha \frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)}{\partial \dot{q}^\alpha} - L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)$$

and a candidate for a momentum variable $\boldsymbol{p}$ through Eq. (4.1.12) but we do not know in general (for arbitrary generalized coordinates) if we can solve Eq. (4.1.12) for $\dot{\boldsymbol{q}}(\boldsymbol{q}, \boldsymbol{p}, t)$ and completely eliminate the $\dot{\boldsymbol{q}}$ in favor of the $\boldsymbol{p}$.

This is the domain of the *Legendre transformation:*

Aside 4.1 – Legendre transformations:

Assume $F(\boldsymbol{x},\boldsymbol{u})$ is C^2 in the components of $\boldsymbol{x}=(x^1,\dots,x^m)^t$, and $\det(\frac{\partial F}{\partial x^i \partial x^j}) \neq 0$. Then the implicit function theorem assures us that the equations

$$y^\alpha = \frac{\partial}{\partial x^\alpha} F(\boldsymbol{x},\boldsymbol{u}) \tag{4.1.14}$$

can be solved locally for the $\boldsymbol{x}$, i.e. there exists a $\boldsymbol{\varphi}$ such that

$$x^\alpha = \varphi^\alpha(\boldsymbol{y},\boldsymbol{u}) \tag{4.1.15}$$

The *Legendre transform* of F is then defined as

$$G(\boldsymbol{y},\boldsymbol{u}) := \mathcal{L}[F](\boldsymbol{y},\boldsymbol{u}) = \boldsymbol{y}\cdot\boldsymbol{\varphi} - F(\boldsymbol{\varphi},\boldsymbol{u}) \tag{4.1.16}$$

such that

$$\frac{\partial G}{\partial y^\alpha} = \varphi^\alpha;\quad \frac{\partial G}{\partial u^i} = -\frac{\partial F}{\partial u^i} \quad\text{and}\quad \det\Big(\frac{\partial^2 G}{\partial y^\alpha \partial y^\beta}\Big)\det\Big(\frac{\partial^2 F}{\partial x^\kappa \partial x^\rho}\Big) = 1 \tag{4.1.17}$$

The transformation is one to one and invertible.

Eq. (4.1.17) can be verified by a direct calculation that only employs the chain rule in various ways:

$$\frac{\partial G}{\partial y^\alpha} = \varphi^\alpha + y^\beta \frac{\partial \varphi^\beta}{\partial y^\alpha} - \frac{\partial F}{\partial \varphi^\beta}\frac{\partial \varphi^\beta}{\partial y^\alpha} = \varphi^\alpha + \left(y^\beta - \frac{\partial F}{\partial \varphi^\beta}\right)\frac{\partial \varphi^\beta}{\partial y^\alpha} \overset{\text{Eq. (4.1.14)}}{=} \varphi^\alpha$$

and, since $\frac{\partial y^\alpha}{\partial u^i} = 0$ by construction

$$\frac{\partial G}{\partial u^\alpha} = y^\beta \frac{\partial \varphi^\beta}{\partial u^i} - \frac{\partial F}{\partial \varphi^\beta}\frac{\partial \varphi^\beta}{\partial u^i} - \frac{\partial F}{\partial u^i} = \left(y^\beta - \frac{\partial F}{\partial \varphi^\beta}\right)\frac{\partial \varphi^\beta}{\partial u^i} - \frac{\partial F}{\partial u^i} \overset{\text{Eq. (4.1.14)}}{=} -\frac{\partial F}{\partial u^i}$$

For our case we identify L with F, $\boldsymbol{x} = \varphi(\boldsymbol{y},\boldsymbol{u}) \leftrightarrow \dot{\boldsymbol{q}}$, $\boldsymbol{u} \leftrightarrow (\boldsymbol{x}^t, t)^t$, and lastly H with G.

The main condition for the existence of the Legendre transformation form L to H becomes

$$\det\Big(\frac{\partial^2 L}{\partial \dot{q}^\alpha \partial \dot{q}^\beta}\Big) \neq 0 \tag{4.1.18}$$

If true, we can express the $\boldsymbol{q}$ in terms of $\boldsymbol{q}$, $\boldsymbol{p}$ and t as $\boldsymbol{q}(\boldsymbol{q},\boldsymbol{p},t)$ so that we obtain the Hamiltonian

$$H(\boldsymbol{q},\boldsymbol{p},t) := \boldsymbol{p}\cdot\dot{\boldsymbol{q}}(\boldsymbol{q},\boldsymbol{p},t) - L(\boldsymbol{q},\dot{\boldsymbol{q}}(\boldsymbol{q},\boldsymbol{p},t),t) \tag{4.1.19}$$

The equations of motion follow directly from Eq. (4.1.17):

$$\dot{q}^\alpha = \frac{\partial H}{\partial p^\alpha},\quad \frac{\partial H}{\partial q^\alpha} = -\frac{\partial L}{\partial q^\alpha} = -\dot{p}^\alpha \quad \det\Big(\frac{\partial^2 H}{\partial \dot{p}^\alpha \partial \dot{p}^\beta}\Big) \neq 0 \tag{4.1.20}$$

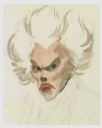
so that we end up with

$$\dot{q}^\alpha = \frac{\partial H}{\partial p^\alpha} \qquad \text{and} \qquad \dot{p}^\alpha = -\frac{\partial H}{\partial q^\alpha} \tag{4.1.21}$$

These are the first order equations of motion for generalized coordinates and momenta, i.e. the generalization of Eqns. (1.7.2) to a form that allows us to include constraints.

They are referred to as *canonical eqations* or *Hamilton's equations of motion*.

From Wikipedia (*much more there*): Adrien-Marie Legendre (18 September 1752 – 10 January 1833) was a French mathematician. Legendre made numerous contributions to mathematics. He is known for the Legendre transformation, which is used to go from the Lagrangian to the Hamiltonian formulation of classical mechanics. In thermodynamics it is also used to obtain the enthalpy and the Helmholtz and Gibbs (free) energies from the internal energy. He is also the namegiver of the Legendre polynomials, solutions to Legendre's differential equation, which occur frequently in physics and engineering applications, e.g. electrostatics.



To the right: 1820 watercolor caricature of Adrien-Marie Legendre by French artist Julien-Leopold Boilly (see portrait debacle), the only existing portrait known.

4.2 Canonical systems

Canonical systems: A mechanical system is said to be a *canonical system* if it admits a Hamiltonian function such that its equations of motion take the form (4.1.21).

Note that every Lagrangian system that fulfils the condition (4.1.18) is canonical. The converse is also true: if $\det(\frac{\partial^2 H}{\partial \dot{p}^\alpha \partial \dot{p}^\beta}) \neq 0$ (viz. (4.1.20)), then every canonical system with f degrees of freedom satisfies the Euler-Lagrange equations for a Lagrangian given as the Legendre transformation of H, i.e.

$$L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) = \mathcal{L}[H](\boldsymbol{q}, \dot{\boldsymbol{q}}, t) = \dot{\boldsymbol{q}} \cdot \boldsymbol{p}(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) - H(\boldsymbol{q}, \boldsymbol{p}(\boldsymbol{q}, \dot{\boldsymbol{q}}, t), t) \tag{4.2.1}$$

A key property of the Legendre transformation is is invertibility, if you can go from one to the other, then you can also go back. If the Legendre transformation exists at all, L and H are completely equivalent.

Remark 4.1 – equivalence of L and H:

The condition on the second derivative tells us that the function to be transformed is either convex or concave. In fact, for the Legendre transformation to exist, the weaker condition of convexity of the function (or its negative) is the essential requirement, not its differentiability. This weaker form is important for other branches of physics, such as thermodynamics of equilibrium states, or quantum field theory.

Examples of canonical systems:

Motion of a particle in a central field: Angular momentum is conserved motion will take place in a plane perpendicualr to $\boldsymbol{l}$. We introduce polar coordinates and write

$$x^1 = r\cos\varphi, \quad x^2 = r\sin\varphi \quad \Rightarrow \quad \boldsymbol{v}^2 = \dot{r}^2 + r^2\dot{\varphi}^2$$

i.e.

$$L = T - U = \frac{m}{2}(\dot{r}^2 + r^2\dot{\varphi}^2) - U(r) \tag{4.2.2}$$

and label $q^1 = r$, $q^2 = \varphi$, to find

$$p^1 = p_r = \frac{\partial L}{\partial \dot{q}^1} = m\dot{r} \quad \text{and} \quad p^2 = p_\varphi = \frac{\partial L}{\partial \dot{q}^2} = \frac{\partial L}{\partial \dot{\varphi}} = mr^2\dot{\varphi} \tag{4.2.3}$$

For the Legendre transformation to work, we need

$$\det\Big(\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}\Big) = \det\begin{pmatrix} m & 0 \\ 0 & mr^2 \end{pmatrix} = m^2 r^2 \neq 0 \quad \text{for } r \neq 0 \tag{4.2.4}$$

The coodinate singularity at $r = 0$ prevents us from performing the Legendre transformation everywhere! Everywhere but at the origin

$$H(\boldsymbol{q}, \boldsymbol{p}) = \frac{p_r^2}{2m} + \frac{p_\varphi^2}{2mr^2} + U(r) \tag{4.2.5}$$

The canonical equations are

$$\dot{r} = \frac{\partial H}{\partial p_r} = \frac{p_r}{m} \qquad \dot{p}_r = -\frac{\partial H}{\partial r} = \frac{p_\varphi^2}{mr^3} - \frac{\partial U}{\partial r} \tag{4.2.6a}$$

$$\dot{\varphi} = \frac{\partial H}{\partial p_\varphi} = \frac{p_\varphi}{mr^2} \qquad \dot{p}_\varphi = 0 \tag{4.2.6b}$$

Indeed $p_\varphi = |\boldsymbol{l}|$ and it is conserved as a cyclical coordinate.

› **A charged particle in electromagnetic fields:** We start from (2.3.34), i.e

$$L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) := \frac{m}{2}\dot{\boldsymbol{q}}^2 - e\Phi(\boldsymbol{q}, t) + e\dot{\boldsymbol{q}} \cdot \boldsymbol{A}(\boldsymbol{q}, t) \tag{4.2.7}$$

We stay in a Cartesian coordinate system an obtain the canonically conjugate momenta as

$$p^i = \frac{\partial L}{\partial \dot{q}^i} = m\dot{q}^i + eA^i(\boldsymbol{q}, t) \tag{4.2.8}$$

which can clearly be solved for $\dot{\boldsymbol{q}}$: $\dot{\boldsymbol{q}} = \frac{\boldsymbol{p}}{m} - \frac{e}{m}\boldsymbol{A}(\boldsymbol{q}, t)$, so that

$$H = \frac{\boldsymbol{p} \cdot \big(\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{q}, t)\big)}{m} - \frac{1}{2m}\Big(\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{q}, t)\Big)^2 + e\Phi + \frac{-e\boldsymbol{A} \cdot \Big(\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{q}, t)\Big)}{m}$$

or

$$H = \frac{1}{2m}\Big(\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{q}, t)\Big)^2 + e\Phi \tag{4.2.9}$$

Here it get's subtle:

- $m\dot{\boldsymbol{q}} = \boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{q}, t)$ is what we call the *kinematic momentum*: We see that in the presence of a vector potential the kinetic energy is not expressed in terms of $\boldsymbol{p}^2$ but in terms of $\big(\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{q}, t)\big)^2$. This is a generic feature related to gauge symmetry a deep concept by itself and deserves its own name.

- Nevertheless, $p^i := \dfrac{\partial L}{\partial \dot{q}^i}$ does not become obsolete, since its role in the Legendre transform between Hamiltonian and Lagrangian remains unaffected. To distinguish it from the kinematic momenutm we call it the momentum *canonically conjugate* to q^i.

5 Symmetries and conservation laws – Noether's theorem

5.1 Motivation

In this section we study autonomous systems with f degrees of freedom with Lagrangian

$$L(\boldsymbol{q},\dot{\boldsymbol{q}}) = T(\boldsymbol{q},\dot{\boldsymbol{q}}) - U(\boldsymbol{q}) \tag{5.1.1}$$

We had already seen at the beginning of Sec. 4.2 that in this case

$$\tilde{H}(\boldsymbol{q},\dot{\boldsymbol{q}}) := \dot{q}^\alpha \frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha} - L(\boldsymbol{q},\dot{\boldsymbol{q}})$$

is a *constant of motion*, i.e. it is conserved for solution of the equations of motion.

$$\frac{d\tilde{H}}{dt} = \ddot{q}^\alpha \frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha} + \dot{q}^\alpha \frac{d}{dt}\frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha} - \frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial q^\alpha}\dot{q}^\alpha - \frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha}\ddot{q}^\alpha = 0$$

(cancel directly: $\ddot{q}^\alpha \frac{\partial L}{\partial \dot{q}^\alpha}$ and $-\frac{\partial L}{\partial \dot{q}^\alpha}\ddot{q}^\alpha$; zero on EOM: $\dot{q}^\alpha \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^\alpha} - \frac{\partial L}{\partial q^\alpha}\dot{q}^\alpha$)

In many of the examples we have seen, this quantity turned out to be the total energy of the system, but this is by no means automatic:

For $\tilde{H}$ to be the energy we need that

$$\tilde{H} = \dot{q}^\alpha \frac{\partial L}{\partial \dot{q}^\alpha} - T + U \overset{!}{=} T + U = E \quad \text{i.e. we need that} \quad \dot{q}^\alpha \frac{\partial L}{\partial \dot{q}^\alpha} = 2T \tag{5.1.2}$$

Eq. (5.1.2) holds if T is a homogeneous function of degree 2 in the $\dot{\boldsymbol{q}}$, i.e. if and only if we take T to be of the form

$$T = t^{\alpha\beta}(\boldsymbol{q})\dot{q}^\alpha \dot{q}^\beta \ . \tag{5.1.3}$$

> **Reminder 5.1 – homogeneous functions of degree n:**
> are simply of the form (summation convention on the i_k!)
>
> $$F(\boldsymbol{x}) = f^{i_1,\dots,i_n} x^{i_1} \cdots x^{i_n} \tag{5.1.4}$$
>
> with $\boldsymbol{x}$-independent (tensor) coefficients $f^{i_1,\dots,i_n}$ (this is often stated differently and very obscurely in the literature).
>
> A straightforward consequence is Euler's theorem on homogeneous functions, which states that
>
> $$x^i \frac{\partial}{\partial x^i} F(\boldsymbol{x}) = nF \tag{5.1.5}$$

which you check by simply direct computation using (??). The real (still not very complicated) issue is the reverse: how to get (5.1.4) from (5.1.5).

One of the key observation in the above is that constants of the motion $f(\boldsymbol{q}, \dot{\boldsymbol{q}})$ are conserved only for solutions of the equations of motion. Any time derivative $\frac{df}{dt}$ that we take is for physical orbits, an *orbital derivative*. It is interesting to note that we did not need to know the solutions to the equations of motion themselves to conclude that the $\tilde{H}$ above was conserved – all we needed what the form of the equations of motion.

A key point in our study of conserved quantities is that we do not need to know the solutions themselves to judge if a quantity is conserved – it is enough to know the form of the equations of motion.

5.2 Noether's theorem

We are again restricting ourselves to an autonomous system with Lagrangian that does not explicitly depend on time:

$$L = L(\boldsymbol{q}, \dot{\boldsymbol{q}}) \tag{5.2.1}$$

Imagine that this Lagrangian possesses *continuous symmetries*, i.e. differentiable one parameter families of maps that take trajectories $\boldsymbol{q}(t)$ into other trajectories

$$h_s(\boldsymbol{q}(t)) \quad \text{with} \quad \boldsymbol{h}_{s=0}(\boldsymbol{q}(t)) = \boldsymbol{q}(t) \tag{5.2.2}$$

for $s \in]s_0, s_1[\ni 0$ such that the Lagrangian remains invariant

$$L(\boldsymbol{q}, \dot{\boldsymbol{q}}) = L(\boldsymbol{h}_s(\boldsymbol{q}(t)), \dot{\boldsymbol{h}}_s(\boldsymbol{q}(t)))$$

or, equivalently

$$L(\boldsymbol{h}_s(\boldsymbol{q}(t)), \dot{\boldsymbol{h}}_s(\boldsymbol{q}(t))) - L(\boldsymbol{q}, \dot{\boldsymbol{q}}) = 0 \qquad \text{for all} \qquad s \in]s_0, s_1[\ni 0 \tag{5.2.3}$$

for all s in our open interval.

with respect to s

These need not be solutions to the equations of motion!

This is why we call it a symmetry!

As a consequence, also the action does not change as we move from one value of s to another. In particular, this implies that if $\boldsymbol{q}(t)$ is a solution to the equations of motion (an extremal point of the action), then so is $\boldsymbol{h}_s(\boldsymbol{q}(t))$: a symmetry takes solutions of the equations of motion into other solutions.

This leads to conserved quantities as we see if we calculate

$$\begin{aligned}
0 = \left.\frac{d}{ds}\right|_0 0 = \left.\frac{d}{ds}\right|_0 \Big(L(\boldsymbol{h}_s(\boldsymbol{q}(t)), \dot{\boldsymbol{h}}_s(\boldsymbol{q}(t))) - L(\boldsymbol{q}, \dot{\boldsymbol{q}}\Big) = \left.\frac{d}{ds}\right|_0 L(\boldsymbol{h}_s(\boldsymbol{q}(t)), \dot{\boldsymbol{h}}_s(\boldsymbol{q}(t))) \\
= \frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial q^\alpha} \left.\frac{dh_s^\alpha(\boldsymbol{q}(t))}{ds}\right|_0 + \frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha} \left.\frac{d\dot{h}_s^\alpha(\boldsymbol{q}(t))}{ds}\right|_0 \\
= \frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial q^\alpha} \left.\frac{dh_s^\alpha(\boldsymbol{q}(t))}{ds}\right|_0 + \frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha} \frac{d}{dt} \left.\frac{dh_s^\alpha(\boldsymbol{q}(t))}{ds}\right|_0
\end{aligned} \tag{5.2.4}$$

Now, let me add and subtract $\left(\frac{d}{dt}\frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha}\right) \left.\frac{dh_s^\alpha(\boldsymbol{q}(t))}{ds}\right|_0$ and group the terms like

$$= \left(\frac{d}{dt}\frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha}\right) \left.\frac{dh_s^\alpha(\boldsymbol{q}(t))}{ds}\right|_0 + \frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha} \frac{d}{dt} \left.\frac{dh_s^\alpha(\boldsymbol{q}(t))}{ds}\right|_0 + \left(\frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial q^\alpha} - \frac{d}{dt}\frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha}\right) \left.\frac{dh_s^\alpha(\boldsymbol{q}(t))}{ds}\right|_0$$

The first two terms assemble into a total derivative and the second term term vanishes on solutions to the equations of motion:

$$= \frac{d}{dt}\left(\frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha}\left.\frac{dh_s^\alpha(\boldsymbol{q}(t))}{ds}\right|_0\right) + \underbrace{\left(\frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial q^\alpha} - \frac{d}{dt}\frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha}\right)}_{\text{zero on EOM}}\left.\frac{dh_s^\alpha(\boldsymbol{q}(t))}{ds}\right|_0 \tag{5.2.5}$$

We have arrived at the first version of Noether's theorem:

Theorem 2 – Noether's theorem for explicit symmetries of the Lagrangian:
Any continuous symmetry of the Lagrangian represented by $h_s(\boldsymbol{q})$ (such that Eq. (5.2.3) holds) leads a quantity that is conserved on solutions $\boldsymbol{q}(t)$ to the equations of motion, an integral of motion, of the form

$$I_{h_s}(\boldsymbol{q},\dot{\boldsymbol{q}}) := \frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha}\left.\frac{dh_s^\alpha(\boldsymbol{q}(t))}{ds}\right|_0 \tag{5.2.6}$$

From Wikipedia (*much more there*): **Amalie Emmy Noether**, German pronunciation: ['nøːtɐ], (23 March 1882 – 14 April 1935) was an influential German mathematician known for her groundbreaking contributions to abstract algebra and theoretical physics. Described by David Hilbert, Albert Einstein and others as the most important woman in the history of mathematics, she revolutionized the theories of rings, fields, and algebras. In physics, Noether's theorem explains the fundamental connection between symmetry and conservation laws.



We note that the quantity $\left.\frac{dh_s^\alpha(\boldsymbol{q}(t))}{ds}\right|_0$ plays a special role in our formulation. It is in fact the only remnant of h_s that enters the conserved quantity:

Generators of a symmetry: Given a symmetry parametrized by a differentiable one parameter family of transformations h_s we call

$$\left.\frac{dh_s^\alpha(\boldsymbol{q}(t))}{ds}\right|_0 \tag{5.2.7}$$

the generator of the symmetry.

This is direct correspondence with the definitions we have encountered for Lie algebras as we will see below.

Below we will also generalize this to the case where the Lagrangian is invariant up to a total time derivative, but before we do this, let us look at the two main examples:

Translation symmetry with constant global translations: Assume an n-particle system to be invariant under translations along some spatial direction $\hat{\eta} \in \mathbb{R}^3$: we have a symmetry of the Lagrangian that for the i-th particle can be expressed via

$$\boldsymbol{h}_{s,i}(\boldsymbol{r}_i) = \boldsymbol{r}_i + s\hat{\boldsymbol{\eta}} \qquad i = 1,\ldots,n \tag{5.2.8}$$

Then the associated conserved quantity is

$$\left.\frac{d}{ds}\right|_0 \boldsymbol{h}_{s,i}(\boldsymbol{r}_i) = \hat{\boldsymbol{\eta}} \qquad \text{and} \qquad I_{\hat{\boldsymbol{\eta}}} = \sum_i m_i \dot{\boldsymbol{r}}_i \cdot \hat{\boldsymbol{\eta}} =: P_\eta \tag{5.2.9}$$

the total momentum in η-direction.

If translations in three linearly independent directions are symmetries, all components of momentum (momentum as a whole is/) are conserved.

› **Rotation symmetry around a fixed axis $\hat{\boldsymbol{\varphi}}$**

$$\boldsymbol{h}_{s,i}(\boldsymbol{r}_i) = R(s\hat{\boldsymbol{\varphi}})\boldsymbol{r}_i \qquad i = 1, \dots, n \tag{5.2.10}$$

so that, in component notation

$$\left.\frac{d}{ds}\right|_0 \boldsymbol{h}_{s,i}(\boldsymbol{r}_i) = \left.\frac{d}{ds}\right|_0 R(s\hat{\boldsymbol{\varphi}}) \cdot \boldsymbol{r}_i = \left.\frac{d}{ds}\right|_0 e^{s\hat{\boldsymbol{\varphi}}^a i t^a} \cdot \boldsymbol{r}_i \ = \hat{\boldsymbol{\varphi}}^a i t^a \cdot \boldsymbol{r}_i \tag{5.2.11}$$

This is a vector in $\mathbb{R}^3$ (one for each particle i). Let me change to component notation and pick the j-th component:

$$\left[\left.\frac{d}{ds}\right|_0 \boldsymbol{h}_{s,i}(\boldsymbol{r}_i)\right]^j = \hat{\boldsymbol{\varphi}}^a [it^a]^{jk} r_i^k = \hat{\boldsymbol{\varphi}}^a \epsilon^{jak} r_i^k = (\hat{\boldsymbol{\varphi}} \times \boldsymbol{r}_i)^j \tag{5.2.12}$$

Then the associated integral of motion is given by

$$I_{\boldsymbol{\varphi}} = \sum_i m_i \dot{\boldsymbol{r}}_i \cdot (\hat{\boldsymbol{\varphi}} \times \boldsymbol{r}_i) = \sum_i m_i \dot{r}_i^k \epsilon^{klm} \hat{\varphi}^l r_i^m = \sum_i \left(\hat{\varphi}^l \epsilon^{lmk} m_i r_i^m \dot{r}_i^k\right) = \hat{\boldsymbol{\varphi}} \cdot \left(\sum_i \boldsymbol{r}_i \times \boldsymbol{p}_i\right) = l_{\hat{\boldsymbol{\varphi}}} \tag{5.2.13}$$

i.e. the total angular momentum in the direction of the rotation axis $\hat{\boldsymbol{\varphi}}$.

If rotations around three linearly independent directions are symmetries, all components of angular momentum (angular momentum as a whole is/) are conserved.

› **Time translation invariance:** At first glance that would appear to lie outside the scope of our tools. A little trick helps to overcome this difficulty:

We make t a coordinate-like variable by introducing an auxiliary variable τ to parametrize both $\boldsymbol{q} = q(\tau)$ and $t = t(\tau)$ and define the Lagrangian

$$\tilde{L}(\boldsymbol{q}, t; \frac{d\boldsymbol{q}}{d\tau}, \frac{dt}{t\tau}) := L(\boldsymbol{q}, \frac{1}{dt/d\tau}\frac{d\boldsymbol{q}}{d\tau}, t)\frac{dt}{d\tau} \tag{5.2.14}$$

In the action integral, this simply amounts to a change of variables, a simple reparametrization of the time axis:

$$S = \int_{t_1}^{t_2} dt \ L = \int_{\tau_1}^{\tau_2} d\tau \ \tilde{L} \tag{5.2.15}$$

Thus S is extremal only if the Lagrange equations that follow from both L and $\tilde{L}$ are fulfilled.

If now L is invariant under time translations

$$\boldsymbol{h}_s(\boldsymbol{q},t)=\begin{pmatrix}\boldsymbol{q}\\ t+s\end{pmatrix}\qquad \left.\frac{d}{ds}\right|_0 \boldsymbol{h}_s(\boldsymbol{q},t)=\begin{pmatrix}0\\1\end{pmatrix} \tag{5.2.16}$$

then so is $\tilde{L}$ and we may apply Noether's theorem to $\tilde{L}$. To this end we set $\boldsymbol{q}=(q^1,\dots,q^f,t=q^{f+1})^t$ and find that

$$I_t=\frac{\partial\tilde{L}}{\partial\dot{q}^\alpha}\left.\frac{d}{ds}\right|_0 h_s^\alpha(\boldsymbol{q},t)=\frac{\partial\tilde{L}}{\partial\dot{q}^{f+1}}\,1=\frac{\partial\tilde{L}}{\partial(dt/d\tau)}=L+\frac{\partial L}{\partial\dot{q}^\alpha}\Big(-\frac{1}{(dt/d\tau)^2}\Big)\frac{dq^\alpha}{d\tau}\frac{dt}{d\tau}=L-\frac{\partial L}{\partial\dot{q}^\alpha}\dot{q}^\alpha \tag{5.2.17}$$

This is $-\tilde{H}$ of Sec 5.1. If the kinetic energy is homogeneous of degree 2 in $\dot{\boldsymbol{q}}$, this becomes the total energy of the system.

5.3 Extending Noether's theorem

We have now covered *constant* translations, rotations and time translations and their associated conserved quantities. This leaves out only one type of transformation that is allowed in the Galilei group of transformations between inertial frames: transformations between frames that move with constant velocity, i.e. translations of the form $\boldsymbol{r}\mapsto\boldsymbol{r}+\boldsymbol{w}t$. Already in the case of the simple n-particle system without potentials we see that this is beyond the scope of theorem 2:

For a system of n free particles with $\boldsymbol{x}:=\begin{pmatrix}\boldsymbol{r}_1\\ \vdots\\ \boldsymbol{r}_n\end{pmatrix}$ and

$$L(\boldsymbol{x},\dot{\boldsymbol{x}})=\sum_i\frac{m_i}{2}\dot{\boldsymbol{r}}_i^2 \tag{5.3.1}$$

Consider now the same system in a different inertial frame $\boldsymbol{x}'$ connected via the the general Galilei-transformation

$$\boldsymbol{x}:=\begin{pmatrix}\boldsymbol{r}_1\\ \vdots\\ \boldsymbol{r}_n\end{pmatrix}\mapsto\boldsymbol{x}':=\begin{pmatrix}R\boldsymbol{r}_1+\boldsymbol{a}+\boldsymbol{w}t\\ \vdots\\ R\boldsymbol{r}_n+\boldsymbol{a}+\boldsymbol{w}t\end{pmatrix}\quad\text{so that}\quad\dot{\boldsymbol{x}}':=\begin{pmatrix}R\dot{\boldsymbol{r}}_1+\boldsymbol{w}\\ \vdots\\ R\dot{\boldsymbol{r}}_n+\boldsymbol{w}\end{pmatrix} \tag{5.3.2}$$

If we had set up the Lagrangian in the primed frame we would have found

$$\begin{aligned}L(\boldsymbol{x}',\dot{\boldsymbol{x}}')&=\sum_i\frac{m_i}{2}\dot{\boldsymbol{r}}_i'^2=\sum_i\frac{m_i}{2}\left(R\dot{\boldsymbol{r}}_i+\boldsymbol{w}\right)^2=\sum_i\frac{m_i}{2}\left(\dot{\boldsymbol{r}}_i^2+2R\dot{\boldsymbol{r}}_i\cdot\boldsymbol{w}+\boldsymbol{w}^2\right)\\&=\sum_i\frac{m_i}{2}\dot{\boldsymbol{r}}_i^2+\frac{d}{dt}\underbrace{\sum_i\left(m_i\boldsymbol{r}_i\cdot(R^{-1}\cdot\boldsymbol{w})+t\frac{m_i}{2}\boldsymbol{w}^2\right)}_{=:M(\boldsymbol{x},t)}\end{aligned} \tag{5.3.3}$$

i.e. the Lagrangian changes by a gauge function $M(\boldsymbol{x},t)$! The culprit for the appearance of the gauge term is a nonzero $\boldsymbol{w}$. This clearly goes beyond our strict invariance requirement of Eq. (5.2.3), yet the equations of motion are not affected, so this does correspond to a symmetry and we expect a conserved quantity to emerge.

Indeed, isolating the $\boldsymbol{w}$-dependence in a one-parameter family of transformations of the form

$$\boldsymbol{h}_s(\boldsymbol{x}) = \begin{pmatrix} r_1 + s\boldsymbol{w}t \\ \vdots \\ r_n + s\boldsymbol{w}t \end{pmatrix} \tag{5.3.4}$$

so that

$$L(\boldsymbol{h}_s(\boldsymbol{x}), \dot{\boldsymbol{h}}_s(\boldsymbol{x})) - L(\boldsymbol{x}, \dot{\boldsymbol{x}}) - \frac{d}{dt} \underbrace{\left(s m_i \boldsymbol{r}_i \cdot \boldsymbol{w} + s^2 t \frac{m_i}{2} \boldsymbol{w}^2 \right)}_{=: M_{\boldsymbol{h}_s}(\boldsymbol{x}, t, s)} = 0 \tag{5.3.5}$$

allows us to again to differentiate this with $\frac{d}{ds}\big|_0$ and look for possible conserved quantities.

For the record: the invariance condition (5.2.3) is now replaced by

$$L(\boldsymbol{h}_s(\boldsymbol{x}), \dot{\boldsymbol{h}}_s(\boldsymbol{x})) - L(\boldsymbol{x}, \dot{\boldsymbol{x}}) - \frac{d}{dt} M_{\boldsymbol{h}_s}(\boldsymbol{x}, t, s) = 0 \tag{5.3.6}$$

with $M_{\boldsymbol{h}_s}(\boldsymbol{x}, t, s)$ a gauge term induced by the symmetry $\boldsymbol{h}_s$.

Retracing our steps from Sec. 5.2 we arrive at

$$0 = \frac{d}{dt} \left(\frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha} \left. \frac{dh_s^\alpha(\boldsymbol{q}(t))}{ds} \right|_0 - \left. \frac{d}{ds} \right|_0 M_{\boldsymbol{h}_s}(\boldsymbol{q}, t, s) \right) + \underbrace{\left(\frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial q^\alpha} - \frac{d}{dt} \frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha} \right)}_{\text{zero on EOM}} \left. \frac{dh_s^\alpha(\boldsymbol{q}(t))}{ds} \right|_0 \tag{5.3.7}$$

Theorem 3 – Noether's theorem for symmetries that generate a gauge term in the Lagrang

Any continuous symmetry of the Lagrangian represented by $h_s(\boldsymbol{q})$ (such that Eq. (5.3.6) holds) leads a quantity that is conserved on solutions $\boldsymbol{q}(t)$ to the equations of motion, an integral of motion, or Noether invariant, of the form

$$I_{h_s}(\boldsymbol{q}, \dot{\boldsymbol{q}}) := \frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \dot{q}^\alpha} \left. \frac{dh_s^\alpha(\boldsymbol{q}(t))}{ds} \right|_0 - \left. \frac{d}{ds} \right|_0 M_{\boldsymbol{h}_s}(\boldsymbol{q}, t, s) \tag{5.3.8}$$

Note that this does not fix normalization: If we wish to connect this to a known quantity with clear physical interpretation, we are allowed to multiply it by any constant.

Center of mass principle: The conserved quantity associated with our motivating example for an n-particle system whose potential is translationally invariant

$$\sum_i (m_i \dot{\boldsymbol{r}}_i \cdot \hat{\boldsymbol{w}} t - m_i \boldsymbol{r}_i \cdot \hat{\boldsymbol{w}}) = (\boldsymbol{p}_{\text{total}} t - m_{\text{total}} \boldsymbol{r}_{\text{cm}}) \cdot \hat{w} \tag{5.3.9}$$

This is nothing but the center of mass principle for the $\hat{\boldsymbol{w}}$-direction, since it implies that ($\boldsymbol{p}_{\text{total}} = m_{\text{total}} \dot{\boldsymbol{r}}_{\text{cm}} = m_{\text{total}} \boldsymbol{v}_{\text{cm}}$)

$$0 = \frac{d}{dt} (m_{\text{total}} \boldsymbol{v}_{\text{cm}} t - m_{\text{total}} \boldsymbol{r}_{\text{cm}}) \cdot \hat{\boldsymbol{w}} \tag{5.3.10}$$

or that the $\hat{\boldsymbol{w}}$ component of $\boldsymbol{v}_{\text{cm}}$ must be constant in time.

6 Elements of mechanics in its phase space formulation

6.1 The general symplectic structure of the canonical equations

Let me define the phase space vector for a system with f degrees of freedom as

$$\boldsymbol{x} = \begin{pmatrix} q^1 \\ \vdots \\ q^f \\ p^1 \\ \vdots \\ p^f \end{pmatrix} \in \mathbb{R}^{2f} \qquad \text{so that} \qquad \boldsymbol{\nabla}_{\boldsymbol{x}} H = \begin{pmatrix} \partial H/\partial q^1 \\ \vdots \\ \partial H/\partial q^f \\ \partial H/\partial p^1 \\ \vdots \\ \partial H/\partial p^f \end{pmatrix} \in \mathbb{R}^{2f} \tag{6.1.1}$$

The canonical equation may then be written as a matrix equation

› **Unified matrix formulation of the canonical equations in phase space:**

$$\dot{\boldsymbol{x}} = \mathbf{J} \cdot \boldsymbol{\nabla}_{\boldsymbol{x}} H \qquad \text{where we have defined} \qquad \mathbf{J} := \begin{pmatrix} \mathbf{0}_{f\times f} & \mathbb{1}_{f\times f} \\ -\mathbb{1}_{f\times f} & \mathbf{0}_{f\times f} \end{pmatrix} \in \mathbb{R}^{2f\times 2f} \tag{6.1.2}$$

The $2f \times 2f$-matrix J swaps the top and bottom halfs of $\boldsymbol{\nabla}_{\boldsymbol{x}} H$ and supplies the minus signs needed in the $\dot{p}^\alpha$-components of the equations so that (6.1.2) indeed is nothing but

$$\begin{pmatrix} \dot{q}^1 \\ \vdots \\ \dot{q}^f \\ \dot{p}^1 \\ \vdots \\ \dot{p}^f \end{pmatrix} = \begin{pmatrix} \partial H/\partial p^1 \\ \vdots \\ \partial H/\partial p^f \\ -\partial H/\partial q^1 \\ \vdots \\ -\partial H/\partial q^f \end{pmatrix} \tag{6.1.3}$$

as intended.

We note that

$$\mathbf{J}^2 = -\mathbb{1} \qquad \text{and} \qquad \mathbf{J}^t = \mathbf{J}^{-1} = -\mathbf{J} \tag{6.1.4}$$

› **Example – The one dimensional harmonic oscillator** ($f = 1$) as described in Sec. 1.8.1 is a prime example, with $\boldsymbol{x} = \boldsymbol{z}$ and $\mathbf{J} = -J$

› **Example – Linear autonomous systems** of with equations of motion of the form

$$\dot{\boldsymbol{x}} = \mathbf{A} \cdot \boldsymbol{x} \tag{6.1.5}$$

where $\mathbf{A}$ is a $2f \times 2f$ matrix, so that we must have

$$\dot{\boldsymbol{x}} = \mathbf{A} \cdot \boldsymbol{x} = \mathbf{J} \boldsymbol{\nabla}_{\boldsymbol{x}} H \tag{6.1.6}$$

or equivalently, using $\mathbf{J}^{-1} = -\mathbf{J}$,

$$-\mathbf{J}\dot{\boldsymbol{x}} = -\mathbf{J}\cdot\mathbf{A}\cdot\boldsymbol{x} = \boldsymbol{\nabla}_{\boldsymbol{x}} H \tag{6.1.7}$$

This is a statement that H must be bilinear in the components of $\boldsymbol{x}$, i.e.

Finish this example!

As in the Lagrangian case we may change coordinates via diffeomorphisms $q^\alpha \mapsto Q^\alpha$ also in our phase space description of mechanics. Since $\boldsymbol{q}$ and $\boldsymbol{p}$ enter the formulation on equal footing we must in fact study *canonical transformations*, diffeomorphisms of coordinates $\{\boldsymbol{q},\boldsymbol{p}\} \mapsto \{\boldsymbol{Q},\boldsymbol{P}\}$, that map $H(\boldsymbol{q},\boldsymbol{p},t) \mapsto H'(\boldsymbol{Q},\boldsymbol{P},t)$ so that the structure of the canonical equations is preserved and we arrive at

$$\dot{q}^\alpha = \frac{\partial H}{\partial p^\alpha} \quad \dot{p}^\alpha = -\frac{\partial H}{\partial q^\alpha} \qquad \Leftrightarrow \qquad \dot{Q}^\alpha = \frac{\partial H'}{\partial P^\alpha} \quad \dot{P}^\alpha = -\frac{\partial H'}{\partial Q^\alpha} \tag{6.1.8}$$

Concepts 6.1 – use canonical transformations to expose conservation laws:

If we can find a canonical transformation that renders some or all new coordinates cyclic we have exposed conservation laws. To do so, we aim at

$$\frac{\partial L}{\partial Q^\alpha} = 0 \tag{6.1.9}$$

for as many α as possible. In this case, also $\frac{\partial H}{\partial Q^\alpha}$ so that

$$\dot{P}^\alpha = -\frac{\partial H}{\partial Q^\alpha} = 0 \tag{6.1.10}$$

so that $\dot{P}^\alpha = a^\alpha = \text{const}$. The system is fully described by

$$H(Q^1,\ldots,Q^{\alpha-1},Q^{\alpha+1},\ldots,Q^f,P^1,\ldots,P^{\alpha-1},a^\alpha,P^{\alpha+1},\ldots,P^f) \tag{6.1.11}$$

In the extreme case that all Q^α are cyclic all $P^\alpha = a^\alpha$ are constant so that

$$\dot{Q}^\alpha = \frac{\partial H}{\partial P^\alpha}\Big|_{P=a} =: v^\alpha(t) \qquad \Rightarrow \qquad Q^\alpha = \int_{t_0}^{t} dt' v^\alpha(t') + b^\alpha \tag{6.1.12}$$

and everything is determined by $2f$ constants of integration, $\{\boldsymbol{a}\}$, $\{\boldsymbol{b}\}$.

Before one can undertake this endeavor it pays to understand what the generic properties of canonical transformations are.

The most efficient way to study canonical transformations uses the unified framework for combined coordinate changes in $\boldsymbol{p}$ and $\boldsymbol{q}$ introduced above in the context of Eq. (6.1.2):

Definition 4 – Canonical transformation:

A diffeomorphism of coordinates $g : \boldsymbol{x} \mapsto \boldsymbol{y}$ (well defined and invertible wherever $\det\left(\frac{\partial x^\alpha}{\partial y^\beta}\right) \neq 0$) that maps $H(\boldsymbol{x}, t) \mapsto H'(\boldsymbol{y}, t)$ according to

$$\begin{array}{ccc} \mathbb{R} & \xrightarrow{\quad \mathrm{id} \quad} & \mathbb{R} \\ H \uparrow & & \uparrow H' \\ \mathbb{R}^{2f} \supset U_1 & \xrightarrow[g]{} & U_2 \subset \mathbb{R}^{2f} \end{array} \qquad H' := \mathrm{id} \circ H \circ g^{-1} = H \circ g^{-1} \tag{6.1.13}$$

so that the structure of the canonical equations is preserved, i.e. so that

$$\dot{\boldsymbol{x}} = \mathbf{J} \cdot \boldsymbol{\nabla}_{\boldsymbol{x}} H(\boldsymbol{x}, t) \qquad \Leftrightarrow \qquad \dot{\boldsymbol{y}} = \mathbf{J} \cdot \boldsymbol{\nabla}_{\boldsymbol{y}} H'(\boldsymbol{y}, t) \tag{6.1.14}$$

is called a *canonical transformation*.

Remark 6.1 – integral form of Eq. (6.1.14):

Instead of requiring Eq. (6.1.14) to hold one may equivalently require that

$$\boldsymbol{p} \cdot \dot{\boldsymbol{q}} - H(q, p, t) \stackrel{!}{=} \boldsymbol{Q} \cdot \dot{\boldsymbol{P}} - H'(Q, P, t) + \frac{d}{dt} M(q, p, Q, P, t) \tag{6.1.15}$$

by appealing to the principle of least action. While conceptually appealing, this is much more indirect and less efficient than working directly with Eq. (6.1.14). C.f. other textbooks such as the classic book by Goldstein.

This equation is what replaces pp121-125 in Scheck. Quite a reduction in effort, don't you think?

To understand what (6.1.14) implies we first note that from Eq. (6.1.13) –by chain rule, and in component notation–

$$\nabla^\alpha_{\boldsymbol{y}} H'(\boldsymbol{y}, t) \stackrel{!}{=} \nabla^\alpha_{\boldsymbol{y}} H(\boldsymbol{x}(\boldsymbol{y}), t) = \nabla^\beta_{\boldsymbol{x}} H(\boldsymbol{x}, t) \frac{\partial x^\beta}{\partial y^\alpha} \ . \tag{6.1.16}$$

This plays a direct role in Eqns (6.1.14), which tell us that

$$\dot{x}^\alpha = \frac{\partial x^\alpha}{\partial y^\beta} \dot{y}^\beta = \frac{\partial x^\alpha}{\partial y^\beta} J^{\beta\gamma} \nabla^\gamma_{\boldsymbol{y}} H'(\boldsymbol{y}, t) \stackrel{(6.1.16)}{=} \frac{\partial x^\alpha}{\partial y^\beta} J^{\beta\gamma} \nabla^\eta_{\boldsymbol{x}} H(\boldsymbol{x}, t) \frac{\partial x^\eta}{\partial y^\gamma} \stackrel{\text{EOM for } \boldsymbol{x}}{=} J^{\alpha\beta} \nabla^\beta_{\boldsymbol{x}} H(\boldsymbol{x}, t) \tag{6.1.17}$$

We note that the last equality imposes a condition on the Jacobian matrix of the transformation that reads

$$\frac{\partial x^\alpha}{\partial y^\beta} J^{\beta\gamma} \frac{\partial x^\eta}{\partial y^\gamma} \stackrel{!}{=} J^{\alpha\beta} \tag{6.1.18}$$

To explore further, we change to matrix notation by setting

$$[\mathbf{M}]^{\alpha\beta} = M^{\alpha\beta} := \frac{\partial x^\alpha}{\partial y^\beta} \qquad \text{so that} \qquad [\mathbf{M}^{-1}]^{\alpha\beta} := \frac{\partial y^\alpha}{\partial x^\beta} \tag{6.1.19}$$

since clearly

$$\delta^{\alpha\beta} = \frac{\partial x^\alpha(y)}{\partial x^\beta} = \frac{\partial x^\alpha}{\partial y^\gamma}\frac{\partial y^\gamma}{\partial x^\beta}$$

and recast (6.1.18) as

$$\mathbf{M}\cdot\mathbf{J}\cdot\mathbf{M}^t = \mathbf{J} \tag{6.1.20}$$

› **Remark 6.2 – canonical transformations in older textbooks:**
To connect with what is done in older textbooks we need to break up $\mathbf{M}$ into sub-blocks according to

$$\mathbf{M} = \begin{pmatrix} \frac{\partial q}{\partial Q} & \frac{\partial q}{\partial P} \\ \frac{\partial p}{\partial Q} & \frac{\partial p}{\partial P} \end{pmatrix} \tag{6.1.21}$$

It is these sub-blocks that are studied separately there. Since this ignores the fact that momenta and coordinates appear on the same footing in the phase space picture, this is more cumbersome, lengthy, and less general than what has been done here.

› **Remark – Generating functions:**
Move generating functions in here

Move generating functions here

Equation (6.1.20) is the core requirement for canonical transformations. Their Jacobians *must* satisfy this condition and thus belong to what is known as the *symplectic group* Sp_{2f} in $2f$-dimensions:

$$\mathsf{Sp}_{2f} := \left\{\mathbf{M}\in\mathbb{R}^{2f\times 2f} | \mathbf{M}\cdot\mathbf{J}\cdot\mathbf{M}^t = \mathbf{J}\right\} \tag{6.1.22}$$

These groups also are matrix Lie groups.

› Sp_{2f} **as a group:** The group nature is easy to see: $\mathbb{1}$ is obviously an element of the set Sp_{2f} and furnishes the neutral element. (Also $\mathbf{J}\in\mathsf{Sp}_{2f}$ as follows from its properties given in (6.1.4)). What is left is to check that it is closed under composition of any two elements $\mathbf{M_1}$ and $\mathbf{M_2}$

$$\mathbf{M}_1\mathbf{M}_2\mathbf{J}(\mathbf{M}_1\mathbf{M}_2)^t = \mathbf{M}_1\mathbf{M}_2\mathbf{J}\mathbf{M}_2^t\mathbf{M}_1^t \overset{\mathbf{M}_2\in\mathsf{Sp}_{2f}}{=} \mathbf{M}_1\mathbf{J}\mathbf{M}_1^t \overset{\mathbf{M}_1\in\mathsf{Sp}_{2f}}{=} \mathbf{J} \tag{6.1.23}$$

and that all elements possess inverses that are group elements themselves. This we verify by *constructing* an inverse from Eq. (6.1.20)

$$\mathbf{M}\cdot\mathbf{J}\cdot\mathbf{M}^t = \mathbf{J} \Leftrightarrow \mathbf{M}\cdot\mathbf{J}\cdot\mathbf{M}^t\mathbf{J}^{-1} = \mathbb{1} \Leftrightarrow \mathbf{J}\cdot\mathbf{M}^t\mathbf{J}^{-1} = \mathbf{M}^{-1} \tag{6.1.24}$$

Alternatively you might do a similarity transform on $\mathbf{M}\cdot\mathbf{J}\cdot\mathbf{M}^t = \mathbf{J}$, (multiplying from the left with $\mathbf{M}^{-1}$ and from the right with $[\mathbf{M}^{-1}]^t = [\mathbf{M}^t]^{-1}$ to get $\mathbf{J} = \mathbf{M}^{-1}\mathbf{J}[\mathbf{M}^{-1}]^t$ which also tells us that $\mathbf{M}^{-1}\in\mathsf{Sp}_{2f}$, but fails to give an explicit expression.

Note that the group condition can be also spelled out differently: Since $\mathbf{M}^{-1} = \mathbf{J}\mathbf{M}^t\mathbf{J}^{-1}$ is a group element, it satisfies

$$(-\mathbf{J}\mathbf{M}^t\mathbf{J})\mathbf{J}(-\mathbf{J}\mathbf{M}^t\mathbf{J})^t = \mathbf{J} \Leftrightarrow \mathbf{J}\mathbf{M}^t\mathbf{J}^3\mathbf{M}\mathbf{J} = \mathbf{J} \Leftrightarrow \mathbf{M}^t\mathbf{J}\mathbf{M} = \mathbf{J} \tag{6.1.25}$$

Carefully count minus signs arising from $\mathbf{J}^2 = -\mathbb{1}$ and $\mathbf{J}^t = -\mathbf{J}$.

The Lie-algebra sp_{2f}: is the set of $\mathbb{R}^{2f\times 2f}$ matrices that satisfy

$$\mathbf{X}\cdot\mathbf{J} + \mathbf{J}\cdot\mathbf{X}^t = 0 \tag{6.1.26}$$

Multiplying by $\mathbf{J}^{-1} = -\mathbf{J}$ from the left this turns into $-\mathbf{J}\cdot\mathbf{X}\cdot\mathbf{J} + \mathbf{X}^t = 0$ which can be decoded by making a block matrix ansatz for $\mathbf{X} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$ for which

$$\mathbf{J}\cdot\mathbf{X}\cdot\mathbf{J} = \begin{pmatrix} C & D \\ -A & -B \end{pmatrix}\cdot\mathbf{J} = \begin{pmatrix} -D & C \\ B & -A \end{pmatrix} \overset{!}{=} \begin{pmatrix} A^t & C^t \\ B^t & D^t \end{pmatrix} \tag{6.1.27}$$

We conclude that $-D = A^t$, $B = B^t$ and $C = C^t$

$$\mathbf{X} = \begin{pmatrix} A & B \\ C & -A^t \end{pmatrix} \tag{6.1.28}$$

The determinant condition imposes $\mathrm{tr}(\mathbf{X}) = 0$, which is already implicit in (6.1.28) and therefore leads to no further restriction on the sub-matrix A.

Analogy with $\mathsf{O}(2f)$ – $\mathbf{J}$ as a non-degenerate skew symmetric bilinear form: Note that the definition of Sp_{2f} reduces to that of $\mathsf{O}(2f)$ if we replace $\mathbf{J} \mapsto \mathbb{1}$. Just as $\mathsf{O}(2f)$ are the matrices that leave the scalar product $\boldsymbol{x}^t\cdot\boldsymbol{y} = \boldsymbol{x}^t\cdot\mathbb{1}\cdot\boldsymbol{y}$ invariant, Sp_{2f} can be interpreted as the set of transformations that leave the skew symmetric *symplectic bilinear* form

$$[\boldsymbol{x},\boldsymbol{y}] := \boldsymbol{x}^t\cdot\mathbf{J}\cdot\boldsymbol{y} \tag{6.1.29}$$

Check that this is linear in both slots.

invariant.

One of the most important properties of $[\boldsymbol{x},\boldsymbol{y}]$ is that if $[\boldsymbol{x},\boldsymbol{y}] = 0$ for all $\boldsymbol{x}$, then $\boldsymbol{y} = 0$ – $[\boldsymbol{x},\boldsymbol{y}]$ (or the matrix $\mathbf{J}$ used to define it) is said to be non-degenerate.

We note that we can use the bracket notation to recast the equations of motion as

$$\dot{x}^\alpha = -[\boldsymbol{\nabla}_{\boldsymbol{x}}H(\boldsymbol{x},t), \boldsymbol{\nabla}_{\boldsymbol{x}}x^\alpha]\ . \tag{6.1.30}$$

Determinant condition: The determinant of every element in Sp_{2f} is $+1$.

The proof of this result uses that the determinant of an arbitrary square matrix A can be rewritten in the form

$$\det\mathbf{A} = \frac{(-1)^{f/2}}{f!\,2^f}\sum_{\pi\in S_{2f}}\mathrm{sign}(\pi)[\boldsymbol{a}^{\pi(1)},\boldsymbol{a}^{\pi(2)}]\cdots[\boldsymbol{a}^{\pi(2f-1)},\boldsymbol{a}^{\pi(2f)}] \tag{6.1.31}$$

See Scheck, p133. This very closely related in spirit to the Leibniz formula for determinants, but does involve $\mathbf{J}$.

where the $\boldsymbol{a}^i$ are the column vectors of the matrix A. Eq. (6.1.31) states that for a sympletic matrix M and an arbitrary matrix $\mathbf{A}$ we get

$$\det(\mathbf{M})\det(\mathbf{A}) = \det(\mathbf{M}\mathbf{A}) \overset{(6.1.31)}{=} \det(\mathbf{A}) \tag{6.1.32}$$

since the columns of $\mathbf{M}\mathbf{A}$ are given by $\mathbf{M}\boldsymbol{a}^i$ and the $[\boldsymbol{x},\boldsymbol{y}]$ on the r.h.s. of (6.1.31) are invariant under $\mathbf{M}\in\mathsf{Sp}_{2f}$. Since this must hold for any $\mathbf{A}$, one concludes $\det\mathbf{M} = 1$.

The determinant condition has a very important consequence for the solutions of Hamilton's equations: we can use it to show that volumes in phase space are preserved by time evolution.

› **Aside 6.1 – symplectic (entymology):**
A calque or loan translation from ancient greek for the latin rooted complex. Complex from *complexus* (com-plectere) "braided together". Previously, the symplectic group had been called the line complex group.

6.2 Preservation of the phase space volumes under time evolution

Let me quote from Sec. 1.9:

" *If we know all solutions corresponding to all possible initial conditions* $\boldsymbol{x}(t, t_0, \boldsymbol{x}_0)$ *we may interpret this as the result of a map*

$$\boldsymbol{x}(t, s, \boldsymbol{y}) =: \Phi_{t,s}(\boldsymbol{y}) \tag{6.2.1}$$

$$\Phi_{t,s} : \mathbb{P} \to \mathbb{P} \tag{6.2.2}$$
$$\boldsymbol{y} \mapsto \boldsymbol{x} \tag{6.2.3}$$

called the flow in phase space. The theorem above assures us that this map is unique and both it and its inverse are differentiable. With the times $r, s, t \in I$ *we then have*

$$\Phi_{t,s} \circ \Phi_{s,r} = \Phi_{t,r} \qquad \Phi_{t,s}^{-1} = \Phi_{s,t} \qquad \Phi_{s,s} = 1$$
$$\frac{\partial}{\partial t}\Phi_{ts} = F_t \circ \Phi_{ts} \qquad F_t := \frac{\partial}{\partial t}\Phi_{ts}\Big|_{s=t} \tag{6.2.4}$$

This ensures that the Φ *form what is know as one parameter groups.* "

Then we can consider the matrix of the differential (in component notation)

$$[\mathbf{d}\boldsymbol{\Phi}_{t,t_0}(\boldsymbol{y})]^{\alpha\beta} = [\mathbf{d}\boldsymbol{x}(t, t_0, \boldsymbol{y})]^{\alpha\beta} := \frac{\partial \Phi^\alpha}{\partial y^\beta} \tag{6.2.5}$$

and verify

› **Theorem 4 – Liouville's Theorem:**
If $\boldsymbol{\Phi}_{t,t_0}(\boldsymbol{x}_0)$ is the flow of the dynamical system $\dot{\boldsymbol{x}} = \mathbf{J} \cdot \boldsymbol{\nabla}_{\boldsymbol{x}} H(x, t)$ (for all $\boldsymbol{x}, t, t_0$ for which it is well defined) then

$$\mathbf{d}\boldsymbol{\Phi}_{t,t_0}(\boldsymbol{x}_0) \in \mathsf{Sp}_{2f} \tag{6.2.6}$$

so that, in particular, $\det(\mathbf{d}\boldsymbol{\Phi}_{t,t_0}(\boldsymbol{x}_0)) = +1$.

The main consequence of this theorem is that phase space volumes remain constant under time evolution:

$$V_{t_0} := \int\limits_{U_{t_0}} d^{2f}y = \int\limits_{U_t} d^{2f}x \, \det(\frac{\partial x}{\partial y}) = \int\limits_{U_t} d^{2f}x \, \det(\mathbf{d\Phi}_{t,t_0}(\boldsymbol{x}_0)) = \int\limits_{U_t} d^{2f}x = V_t \tag{6.2.7}$$

What is missing is the proof of Eq. (6.2.6):

› **Proof 1 – Proof of Liouville's theorem:**

First observe that at $t = t_0$ we have nothing to prove since obviously the volume is not changing whithout time evolution. Differentially this can be phrased as

$$\mathbf{d\nabla}_{\boldsymbol{x}} H(\mathbf{\Phi}_{t=t_0,t_0}(\boldsymbol{x}_0), t) = \mathbb{1} \in \mathsf{Sp}_{2f} \quad \text{or as} \quad (\mathbf{d\Phi}_{t=t_0,t_0}(\boldsymbol{x}_0))^t \cdot \mathbf{J} \cdot (\mathbf{d\Phi}_{t=t_0,t_0}(\boldsymbol{x}_0)) = \mathbf{J} \tag{6.2.8}$$

where I have used the alternative condition of Eq. (6.1.25) since it plays more directly to what follows:

What we need to see is that this remains to be the case as time evolves. Time evolution is goverened by the equation of motion (recall the defintion of flow as the solution obtained from a specific initial condition)

$$\frac{d}{dt}\mathbf{\Phi}_{t,t_0}(\boldsymbol{x}_0) = \mathbf{J} \cdot \boldsymbol{\nabla}_{\boldsymbol{x}} H(\mathbf{\Phi}_{t,t_0}(\boldsymbol{x}_0), t) \tag{6.2.9}$$

Taking the differential of this equation (using the chain rule) we arrive at

$$\frac{d}{dt}\mathbf{d\Phi}_{t,t_0}(\boldsymbol{x}_0) = \mathbf{J} \cdot \mathbf{d\nabla}_{\boldsymbol{x}} H(\mathbf{\Phi}_{t,t_0}(\boldsymbol{x}_0), t) \cdot \mathbf{d\Phi}_{t,t_0}(\boldsymbol{x}_0) \tag{6.2.10}$$

Transposing this we find

$$\frac{d}{dt}(\mathbf{d\Phi}_{t,t_0}(\boldsymbol{x}_0))^t = -(\mathbf{d\Phi}_{t,t_0}(\boldsymbol{x}_0))^t \cdot (\mathbf{d\nabla}_{\boldsymbol{x}} H(\mathbf{\Phi}_{t,t_0}(\boldsymbol{x}_0), t))^t \cdot \mathbf{J} \tag{6.2.11}$$

This allows us to calculate the time derivative of $(\mathbf{d\Phi}_{t,t_0}(\boldsymbol{x}_0))^t \cdot \mathbf{J} \cdot (\mathbf{d\Phi}_{t,t_0}(\boldsymbol{x}_0))$ by product rule:

$$\begin{aligned}
&\frac{d}{dt}\Big((\mathbf{d\Phi}_{t,t_0}(\boldsymbol{x}_0))^t \cdot \mathbf{J}(\cdot\mathbf{d\Phi}_{t,t_0}(\boldsymbol{x}_0))\Big) \\
&= -(\mathbf{d\Phi}_{t,t_0}(\boldsymbol{x}_0))^t \cdot (\mathbf{d\nabla}_{\boldsymbol{x}} H(\mathbf{\Phi}_{t,t_0}(\boldsymbol{x}_0), t))^t \cdot \mathbf{J} \cdot \mathbf{J} \cdot (\mathbf{d\Phi}_{t,t_0}(\boldsymbol{x}_0)) \\
&\quad + (\mathbf{d\Phi}_{t,t_0}(\boldsymbol{x}_0))^t \cdot \mathbf{J} \cdot \mathbf{J} \cdot (\mathbf{d\nabla}_{\boldsymbol{x}} H(\mathbf{\Phi}_{t,t_0}(\boldsymbol{x}_0), t)) \cdot (\mathbf{d\Phi}_{t,t_0}(\boldsymbol{x}_0)) \\
&= (\mathbf{d\Phi}_{t,t_0}(\boldsymbol{x}_0))^t \cdot \underbrace{\Big((\mathbf{d\nabla}_{\boldsymbol{x}} H(\mathbf{\Phi}_{t,t_0}(\boldsymbol{x}_0), t))^t - (\mathbf{d\nabla}_{\boldsymbol{x}} H(\mathbf{\Phi}_{t,t_0}(\boldsymbol{x}_0), t))\Big)}_{=0 \text{ see } (6.2.13)} \cdot (\mathbf{d\Phi}_{t,t_0}(\boldsymbol{x}_0)) = 0
\end{aligned} \tag{6.2.12}$$

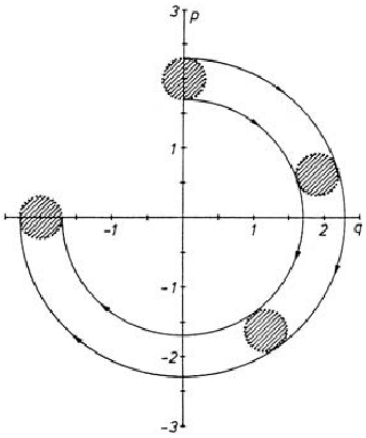
Here we have used that $\mathbf{d\nabla}_{\boldsymbol{x}} H(\mathbf{\Phi}_{t,t_0}(\boldsymbol{x}_0), t)$ is a symmetric matrix, since in fact

$$[\mathbf{d\nabla}_{\boldsymbol{x}} H(\mathbf{\Phi}_{t,t_0}(\boldsymbol{x}_0), t)]^{\alpha\beta} = \frac{\partial^2 H(\boldsymbol{x}(\boldsymbol{x}_0), t)}{\partial x^\alpha \partial x^\beta} \tag{6.}$$

Eq. (6.2.8) provides the initial condition, Eq. (6.2.12) ensures that it remains in Sp_{2f} at all t. QED

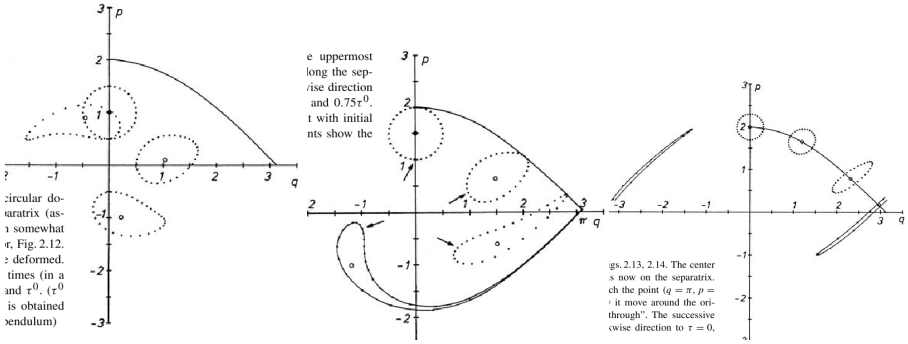
› **Examples:**

- **Harmonic oscillator:** Here everything is fully apparent from the full solutions obtained in Sec. 1.8.1. Even the shape of the volume is retained, no matter what the intitial conditions:



Fix graphics

- **The mathematical pendulum** is more complicated, the volumes get deformed since the behavior near the separatrix is special



Fix graphics 3 times

6.3 Poisson brackets as a realization of the symplectic bilinear form for phase space gradients

The Poisson bracket is a skew symmetric bilinear of derivatives of two dynamical quantities with respect to coordinates and momenta. A dynamical quantity is any physically relevant function of generalized coordinates and momenta such as the kinetic energy, the Hamiltonian function, or the total angular momentum. Let $g(q, p, t)$ be such a dynamical quantity. The Poisson bracket of g and the Hamiltonian function appear in quite a natural way if we calculate the total time change of g along a physical orbit in phase space, as follows:

$$\frac{dg}{dt} = \frac{\partial g}{\partial t} + \frac{\partial g}{\partial q^\alpha}\dot{q}^\alpha + \frac{\partial g}{\partial p^\alpha}\dot{p}^\alpha = \frac{\partial g}{\partial t} + \underbrace{\frac{\partial g}{\partial q^\alpha}\frac{\partial H}{\partial p^\alpha} - \frac{\partial g}{\partial p^\alpha}\frac{\partial H}{\partial q^\alpha}}_{=:\{H,g\}}$$

where the last step includes the definition of the Poisson bracket

$$\{H, g\} := \frac{\partial g}{\partial q^\alpha}\frac{\partial H}{\partial p^\alpha} - \frac{\partial g}{\partial p^\alpha}\frac{\partial H}{\partial q^\alpha} \tag{6.3.1}$$

so that

$$\frac{dg}{dt} = \frac{\partial g}{\partial t} + \{H, g\} \tag{6.3.2}$$

This equation foreshadows the structure of the quantum mechanical time evolution equation for operators in the Heisenberg picture.

The physics statement in Eq. (6.3.2) is that the Hamiltonian governs the dynamical aspects of time evolution, the aspects not governed by an explicit "externally prescribed" time dependence.

Note that Eq. (6.3.2) also applies to $\boldsymbol{q}$ and $\boldsymbol{p}$ themselves (they clearly are observables themselves):

$$\dot{q}^\alpha = \frac{\partial H}{\partial p^\alpha} = \{H, q^\alpha\} \qquad \dot{p}^\alpha = -\frac{\partial H}{\partial q^\alpha} = \{H, p^\alpha\} \tag{6.3.3}$$

Its importance in classical mechanics is widespread:

› **The Poisson bracket in terms of the symplectic bracket of gradients and consequences:**

This is again most easily seen in the unified notation of 6.1: Writing the summation signs explicitly to be able to track summation ranges reliably, we note that

$$\begin{aligned}\{a, b\} :=& \sum_{\alpha=1}^{f} \left(\frac{\partial b}{\partial q^\alpha} \frac{\partial a}{\partial p^\alpha} - \frac{\partial b}{\partial p^\alpha} \frac{\partial a}{\partial q^\alpha} \right) = \sum_{\alpha,\beta=1}^{f} \left(\frac{\partial b}{\partial q^\alpha} \delta^{\alpha\beta} \frac{\partial a}{\partial p^\beta} + \frac{\partial b}{\partial p^\alpha} (-\delta^{\alpha\beta}) \frac{\partial a}{\partial q^\beta} \right) \\ =& \sum_{\alpha,\beta=1}^{2f} - (\nabla_{\boldsymbol{x}}^\alpha a) J^{\alpha\beta} (\nabla_{\boldsymbol{x}}^\beta b)\end{aligned}$$

or

$$\{a, b\} = - (\boldsymbol{\nabla}_{\boldsymbol{x}} a)^t \cdot \mathbf{J} \cdot (\boldsymbol{\nabla}_{\boldsymbol{x}} b) = -[\boldsymbol{\nabla}_{\boldsymbol{x}} a, \boldsymbol{\nabla}_{\boldsymbol{x}} b] \tag{6.3.4}$$

We read off that the Poisson bracket of two observables is minus the symplectic bracket of the phase space gradients of the two observables.

The two equations (6.3.3) are a special case again:

$$\dot{x}^\alpha = -[\boldsymbol{\nabla}_{\boldsymbol{x}} H, \boldsymbol{\nabla}_{\boldsymbol{x}} x^\alpha] \tag{6.3.5}$$

The symplectic bracket notation lends itsself to further observations:

Trivial – entymology: that which I already know (hopefully not missing the ending: how to explain to others).

- **Product rule of the Posisson bracket:**

$$\{a, bc\} = -[\boldsymbol{\nabla}_{\boldsymbol{x}} a, \boldsymbol{\nabla}_{\boldsymbol{x}} (bc)] = -[\boldsymbol{\nabla}_{\boldsymbol{x}} a, \boldsymbol{\nabla}_{\boldsymbol{x}} b] c - [\boldsymbol{\nabla}_{\boldsymbol{x}} a, \boldsymbol{\nabla}_{\boldsymbol{x}} c] b = \{a, b\} c + \{a, c\} b \tag{6.3.6}$$

- **The Poisson bracket is compatible with canonical transformations:** Eq. (6.3.4) makes it trivial to show that the Poisson bracket is conserved under canonical transformations. All we need to know, is that the gradient of a scalar observable transforms just like the Hamiltonian in Eq. (6.1.16):

$$\nabla_{\boldsymbol{y}}^\alpha a'(\boldsymbol{y}, t) \stackrel{!}{=} \nabla_{\boldsymbol{y}}^\alpha a(\boldsymbol{x}(\boldsymbol{y}), t) = \nabla_{\boldsymbol{x}}^\beta a(\boldsymbol{x}, t) \frac{\partial x^\beta}{\partial y^\alpha}$$

or in matrix/vector form

$$\boldsymbol{\nabla}_{\boldsymbol{y}} a'(\boldsymbol{y},t) = \mathbf{M}^t \cdot \boldsymbol{\nabla}_{\boldsymbol{x}} a(\boldsymbol{x},t) \tag{6.3.7}$$

so that

$$\begin{aligned}\{a',b'\} &= -\left(\nabla_{\boldsymbol{y}} a'(\boldsymbol{y},t)\right)^t \cdot \mathbf{J} \cdot \left(\nabla_{\boldsymbol{y}} b'(\boldsymbol{y},t)\right) = -(\mathbf{M}^t \boldsymbol{\nabla}^\beta_{\boldsymbol{x}} a(\boldsymbol{x},t))^t \cdot \mathbf{J} \cdot (\mathbf{M}^t \cdot \boldsymbol{\nabla}^\beta_{\boldsymbol{x}} b(\boldsymbol{x},t) \\ &= -\left(\boldsymbol{\nabla}^\beta_{\boldsymbol{x}} a(\boldsymbol{x},t)\right)^t \cdot \underbrace{\mathbf{M} \cdot \mathbf{J} \cdot \mathbf{M}^t}_{\mathbf{J}} \cdot \boldsymbol{\nabla}^\beta_{\boldsymbol{x}} b(\boldsymbol{x},t) = \{a,b\}\end{aligned} \tag{6.3.8}$$

This is it. Clearly the modern notation of Sec. 6.1 proves its value again.

- **Canonical transformations defined via Poisson brackets:** A transformation is canonical, precisely if

$$\{P^\alpha, Q^\beta\}_{p,q} \stackrel{!}{=} \delta^{\alpha\beta} \qquad \{Q^\alpha, Q^\beta\}_{p,q} \stackrel{!}{=} 0 \qquad \{P^\alpha, P^\beta\}_{p,q} \stackrel{!}{=} 0 \tag{6.3.9}$$

In symplectic notation eq. (6.3.9) is nothing but

$$[\boldsymbol{\nabla}_{\boldsymbol{x}} y^\alpha, \boldsymbol{\nabla}_{\boldsymbol{x}} y^\beta] \stackrel{!}{=} J^{\alpha\beta} \tag{6.3.10}$$

Indeed, if we evaluate the brackets we find

$$[\boldsymbol{\nabla}_{\boldsymbol{x}} y^\alpha, \boldsymbol{\nabla}_{\boldsymbol{x}} y^\beta] = [\mathbf{M}^{-1}]^{\alpha\eta} J^{\eta\kappa} [\mathbf{M}^{-1}]^{\beta\kappa} = J^{\alpha\beta} \Leftrightarrow \mathbf{M}^{-1} \cdot \mathbf{J} \cdot [\mathbf{M}^{-1}]^t \stackrel{!}{=} \mathbf{J} \tag{6.3.11}$$

i.e. the defining relation of canonical transformations, Eq. (6.1.20), only written for $\mathbf{M}^{-1}$ instead of $\mathbf{M}$.

Poisson brackets of coordinates and observables in a given coordinate system

It is a matter of a simple calculation to check that

$$\{q^\alpha, q^\beta\}_{p,q} = 0\ ; \qquad \{p^\alpha, p^\beta\}_{p,q} = 0\ ; \qquad \{p^\alpha, q^\alpha\}_{p,q} = \delta^{\alpha\beta}\ . \tag{6.3.12}$$

This is the classical version of the quantum mechanical commutators of these quantities. In fact this can be viewed as the semiclassical limit of the corresponding quantum condition.

> **Remark 6.3 – connection with QM/QFT:**
> This will remind you strikingly of canonical commutation relations once you encounter them in quantum mechanics or quantum field theory.

For general observables we find

$$\{g, q^\alpha\} = \frac{\partial g}{\partial q^\alpha}\ , \{g, p^\alpha\} = -\frac{\partial g}{\partial p^\alpha} \tag{6.3.13}$$

in a generalization of what what we see for $g = H$

The Jacobi identity: Fill in

The Poisson bracket of two conserved quantities is again a conserved quantity: This makes it a useful theoretical tool to study conservation laws. The trick is to find a full set of *independent* conserved quantities.

The notions developed here again have many parallels in quantum mechanics. Work this out explicitly

From wikipedia (*much more there*): Siméon Denis Poisson (21 June 1781 – 25 April 1840), was a French mathematician, geometer, and physicist. He obtained many important results, but within the elite Académie des Sciences he also was the final leading opponent of the wave theory of light and was proven wrong on that matter by Augustin-Jean Fresnel.



From wikipedia (*much more there*): Joseph Liouville (24 March 1809 – 8 September 1882) was a French mathematician.
Liouville worked in a number of different fields in mathematics, including number theory, complex analysis, differential geometry and topology, but also mathematical physics and even astronomy. He is remembered particularly for Liouville's theorem, a nowadays rather basic result in complex analysis. In number theory, he was the first to prove the existence of transcendental numbers by a construction using continued fractions (Liouville numbers). In mathematical physics, Liouville made two fundamental contributions: the Sturm–Liouville theory, which was joint work with Charles François Sturm, and is now a standard procedure to solve certain types of integral equations by developing into eigenfunctions, and the fact (also known as Liouville's theorem) that time evolution is measure preserving for a Hamiltonian system. In Hamiltonian dynamics, Liouville also introduced the notion of action-angle variables as a description of completely integrable systems. The modern formulation of this is sometimes called the Liouville-Arnold theorem, and the underlying concept of integrability is referred to as Liouville integrability.



7 Outlook – there is more to classical mechanics

- The motion of rigid bodies: Rigid bodies exemplify systems with a very special type of constraint: the relative positions of atoms in a rigid body are very much constrained. This can get quite challenging as already the mathematical analysis of a spinning top reveals.

  This has direct applications to the steering or stabilizing of tumbling satellites if you want more expensive toys.

- Deterministic chaos and deterministic chaotic mechanical systems, where we study system in which directories diverge strongly if we change initial conditions only minutely. (This is to do with a very generalized type of stability analysis.)

- Classical mechanics near the speed of light: special relativity in mechanics.

- A description using the mathematical language of differentiable manifolds is well suited to also incorporate non-holonomic constraints on phase space.

A Symmetries on phase space

A.1 Generalizing the Galilei group to phase space

Bargmann group, central extensions

A.2 The O(4) symmetry of the Kepler problem

- This symmetry is often called a "hidden symmetry" or a "dynamical symmetry", since it does not manifest on configuration space. What it really is is a symmetry on the phase space of the Kepler problem.
- The most concise introduction to the origin of the Runge-Lenz vector in classical mechaincs I know of can be found in Schiff [17, chapter 30]
- Of course there is a stackexchange ref [18] with a few hints at Gilmore[19, chapter 14]:

  "In the book of Gilmore (see previous comment), there is a discussion. One notices, that, in the momentum space, which is in a plane, momenta obey a circle equation. The next observation is that a circle in R3 is promoted to a circle in S3 (included in R4), by a projective transformation, which is a stereographic projection, which is invertible and preserve angles (conformal), so that circles in R3 are in one-to-one correspondence with circles in S3. Now, obviously, SO(4) is a symmetry of S3, so it is also a hidden (dynamical) symmetry of the hydrogenoid atom."

  The word "dynamical" says it all: it is not a symmetry in configuration space but one in the phase space of the problem!

  Gilmore has a nice derivation of Runge-Lenz

  Addintional discussion on stackexchange[20] with a reference to a Fradkin paper[21] that has a surprise in store: **There is an so(4) and su(3) symmetry for all central potential problems**.

  This goes further: As pointed out in the introduction of [22] (also other references e.g. [23] that discovered the same as Fradkin and many more) What the introduction points out and emphasizes is that the symmetries are infinitesimal, those of Lie-algebras, and they do not necessarily integrate to the respective groups. The paper shows that the vectors become multivalued in most cases. I do not see an attempt at constructing the full group and associated invariant subspaces.

- Souriau[24] has an interesting remark on Kepler manifolds in this introduction. There is more on this in chapter 12 (pp121), at the beginning of the chapter "Mechanics".

  Compare this with Gilmore!

  Vivarelli's article on the Kepler problem [25] appears to be reasonably geometrical

B Mathematical aside – $\mathfrak{C}$ and $T\mathfrak{C}$: configuration space and phase space as mathematical objects

B.1 Concepts

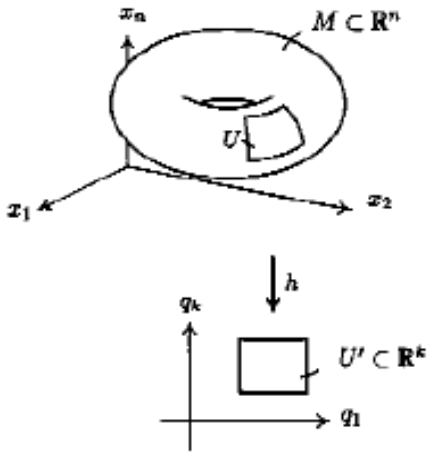
B.1.1 Manifolds and sub-manifolds

› **n-dimensional manifold:** An n-dimensional (topological) *manifold* M is a Hausdorff space with countable basis for its topology that is *locally Euclidean.* in the sense that for each point $p \in M$ there is an open set $U \ni p$ and a invertible continuous map $h : U \to U' = h(U) \in \mathbb{R}^n$. Such a invertible continuous map (homeomorphism) (h, U) is called an *(inner) chart* of M or a local coordinate system of M near p.

The topological statement is needed to have access to the notion of continuous maps.

This is mathematics, the phrase "map" is already taken.

Fix Graphics

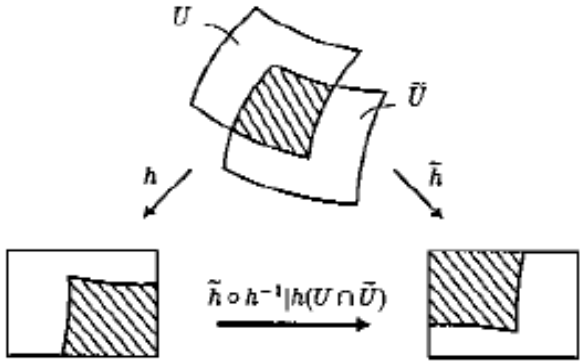


A collection of such maps $\{(h_i, U_i) | \lambda \in \Lambda\}$ (Λ some index set) is called an atlas of M if $\bigcup_{i \in \Lambda} U_i$ covers all of M.

In terms of its coordinate systems, i.e. locally within a U_i, such a manifold "looks" like the Euclidean space $\mathbb{R}^n$.

› **Change of coordinates:**

Fix Graphics



Suppose (h_i, U_i) and $(h_j, \tilde{U}_j)$ are both coordinate systems for M and $U_i \cap U_j \neq \{\}$. They then allow to construct the map

$$h_{ij} := h_j \circ h_i^{-1} : h_i(U_i \cap U_j) \to h_j(U_i \cap U_j) \tag{B.1.1}$$

which describes the change of coordinates on the open set $h_i(U_i \cap U_j)$ (where both sets of coordinates are simultaneously defined).

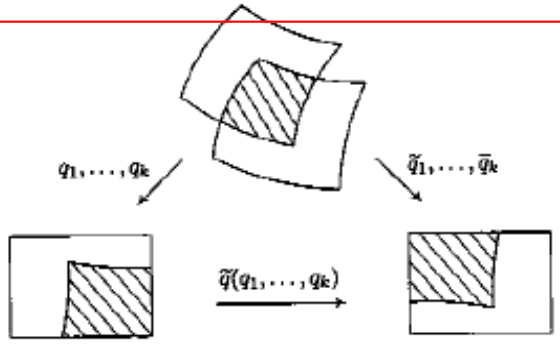
Evidently

$$h_{ii} = \mathrm{id}_{U_i'}, \qquad h_{ij} \circ h_{ki} = h_{kj}, \qquad \text{so that} \qquad h_{ij} = h_{ji}^{-1} \tag{B.1.2}$$

everywhere where the individual maps are defined.

This situation is often encountered in physics applications, the open sets are likely not mentioned, only the coordinates are listed:

Fix Graphics



› **Differentiable atlas:** An atlas is a C^n *atlas* if all its changes of coordinates are C^n, a *differentiable atlas* has all changes of coordinates C^∞.

We can often extend a C^n-atlas by adding suitable coordinate systems but there exists a unique maximal C^n atlas $\mathfrak{D}(\{(h_i, U_i)|\lambda \in \Lambda\})$ for a given C^n-atlas $\{(h_i, U_i)|\lambda \in \Lambda\}$.

The big idea here that differentiability of the atlas is phrased in terms of differentiability of functions between open sets in $\mathbb{R}^n$ where we know how to deal with such notions. This same idea applies to defining differentiable maps between manifolds:

$$\begin{array}{ccc} M \supset U \ni p & \xrightarrow{\quad f \quad} & f(p) \in V \subset N \\ \Big\downarrow h & & \Big\downarrow k \\ \mathbb{R}^n & \xrightarrow[k \circ f \circ h^{-1}]{} & \mathbb{R}^n \end{array} \tag{B.1.3}$$

› **Differentiable maps:** Maps between two differentiable manifolds are called differentiable for two suitable charts the map $k \circ f \circ h^{-1}$ is differentiable in the usual sense.

These can usually be generalized to $\mathbb{R}^n$ in various ways.

› **The simplest example for a manifold is $\mathbb{R}^n$:** $\mathbb{R}^n$ is a differentiable (or C^n) manifold with an atlas generated by the identity map $\mathbf{id} : \mathbb{R}^n \to \mathbb{R}^n$.

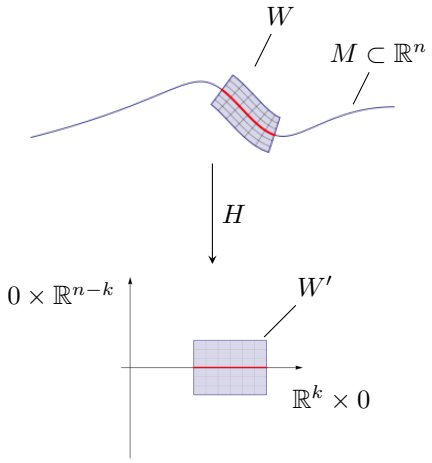
For $\mathbb{R}^3$, this atlas contains all of the curvilinear coordinates systems you might have encountered before like spherical, cylindrical or parabolic coordinates (all locally orthonormal coordinates defined on most of $\mathbb{R}^n$ – they really form charts defined on open subsets of $\mathbb{R}^3$.)

The literature is not completely unified on this issues, sometimes a hypersurface is considered a sub-manifold with $k = n - 1$ only.

› **Sub-manifolds of $\mathbb{R}^n$:**

A subset $M \subset \mathbb{R}^n$ is called a k-dimensional sub-manifold or a k-dimensional hypersurface, if for every point $p \in M$, there is an open set $W \subset \mathbb{R}^n$ around it and a diffeomorphism $H : W \xrightarrow{\cong} W'$ such that

$$H(M \cap W) = (\mathbb{R}^k \times 0) \cap W' \tag{B.1.4}$$



$M \cap W$ and its image are marked in red

In words: what H does is to "straighten out" M and to provide Cartesian coordinates for it – we might call it a local *straightener* for M.

Note that this construction is different from the inner charts introduced in our general definition above since it talks about points inside as well as outside of M. However, H also supplies an inner chart, simply by restriction:

$$\underbrace{H|M \cap W}_{h} : \underbrace{M \cap W}_{U \subset M} \xrightarrow{\cong} \underbrace{(\mathbb{R}^k \times 0) \cap W'}_{U' \subset \mathbb{R}^n}$$

so that

$$h : U \xrightarrow{\cong} U' \tag{B.1.5}$$

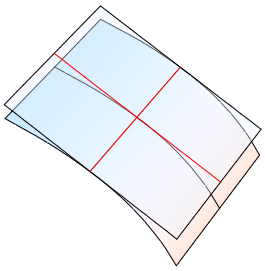
has all the hallmarks of an inner chart for M in the original sense.

Clearly, this becomes a C^n or a differential manifold if we can assemble an appropriate atlas from the (h, U) for all $p \in M$.

B.1.2 Analysis with constraints – tangent bundles and the like

Tangent space and normal space

To deal with local approximations to curved manifolds and more specifically, sub-manifolds in $\mathbb{R}^n$, we need linear approximations to those space. That is the purpose of T_pM the *tangent space* to M at a point $p \in M$. Intuitively:



C Symplectic manifolds

C.1 Gathering input

C.1.1 A quick characterization from stackexchange

A nice summary where the symplectic form comes from at stackexchange:

So, in classical mechanics, we know nothing of this strange "spacetime" and its metric. We know only that systems are described by n continuous generalized coordinates q^i with a certain range, and we take the manifold $\mathcal{M}$ consisting of all possible different $\vec{q}$ as our starting point. Note that there is no metric, no form, nothing on this.

We now include the *generalized momenta* p_i at any point as elements of the cotangent space at that point, and henceforth call the cotangent bundle our *phase space* $\mathcal{P} := T^*\mathcal{M}$.

Now, on the cotangent bundle, there is the tautological one-form $\theta : \mathcal{P} \to T^*\mathcal{P}$. It is uniquely characterized to be the form that *undoes* the pullback β^* by $\beta : \mathcal{M} \to T^*\mathcal{M}$ on the coordinate manifold by $\beta^*\theta = \beta$. It is *natural* in the sense that it is characterized by an universal property and always exists *uniquely*. In coordinates, it is $\theta = p_i \mathrm{d}q^i$.

From this, the symplectic form simply arises as $\omega := \mathrm{d}\theta$. As θ was natural, so is ω, and the proof that ω is symplectic is simply that it is locally given by $\omega = \mathrm{d}p_i \wedge \mathrm{d}q^i$, which is obviously a symplectic form on $\mathbb{R}^n \times \mathbb{R}^n$

So, we do not *choose* a symplectic form, there is one, and only one, natural candidate. Note that *there is no such candidate for a metric.*

If we are now given an "energy function" - the Hamiltonian H - on $\mathcal{P}$, it turns out that demanding that $\theta(X_H)$ be the action reproduces Hamilton's equations, which, by their equivalence to Lagrangian/Newtonian mechanics, are the *correct* equations of motions. Furthermore, the symplectic form gives the correct way to implement the Poisson bracket (which is antisymmetric, and which a metric could never do) by

$$\{f, g\} := \omega(X_f, X_g)$$

where X_f is the vector field defined by a differentiable function $f : \mathcal{P} \to \mathbb{R}$ through $\mathrm{d}f \overset{!}{=} \omega(X_f, \cdot)$.

One can also show now that this is really a Poisson bracket and derive the time evolution equation on the phase space for observables, but I believe this is sufficient to be convincing that the symplectic structure is indeed the *natural* setting for Hamiltonian mechanics.

Lastly, and somewhat unrelated, we note that, on Riemannian manifolds, it is quite possible to consider the geodesics as a Hamiltonian flow, where the Hamiltonian is defined by the metric, but we *still* use the symplectic cotangent bundle to define the flow *on*.

C.1.2 Candidates for literature

- Paulette Libermann, Charles-Michel Marle "Symplectic Geometry and Analytical Mechanics" [26]
- Ana Cannas da Silva "Lectures on Symplectic Geometry" [27] also looks very nice. Free pdf available.
- H. Hofer and E. Zehnder, Symplectic Invariants and Hamiltonian Dynamics. [28]. Looks very readable.

› J.-M. Souriau, “Structure of dynamical systems : a symplectic view of physics” [24] would appear to be a classic

C.2 Solving Kepler via quaternions – a little math excursion

A nice little representation of space and the rotations on it often used in writing efficient computer graphics code uses quaternions to represent space. This is based on Vrbik[29].

C.3 Applications of elliptic functions

This is a topic that has been exorcised from classical mechanics text, I would presume largely for reasons of time. The result is that students going through a modern curriculum are left with a notion of the mysterious and complicated that ties in with what is probably the first opportunity for a first contact with special functions.

There are many more applications of elliptic functions in physics that go far beyond classical mechanics where an early contact with the material might have helped to remove a barrier to material that is not too complicated to be taught early on.

I have three main sources to recommend:

- A very pedagocical introduction is presented in William A Schwalm's "Lectures on Selected Topics in Mathematical Physics: Elliptic Functions and Elliptic Integrals" [30]
- A shorter introduction is Alain J. Brizard "A primer on elliptic functions with applications in classical mechanics" [31]
- Still pedagogical but a little deeper is "Elliptic Functions and Elliptic Integrals" by Viktor Prasolov and Yuri Solovyev [32].

You will find a wealth of applications, from the anharmonic pendulum, the mathematical and spherical penculum to couple pendula in the form of the sine-Gordon equation, the solitons of the Korteweg De Vries equation

Bibliography

[1] F. Scheck, *Mechanics, From Newton's laws to determinitic chaos*. Springer-Verlag GmbH, 2018. (document)

[2] F. H. B. Tom W. B. Kibble, *Classical Mechanics (5th Edition)*. Imperial College Press, 2004. (document)

[3] H. Goldstein, *Classical mechanics*. Addison Wesley, San Francisco, 2002. (document)

[4] A. Beléndez, C. Pascual, D. Méndez, T. Beléndez and C. Neipp, *Exact solution for the nonlinear pendulum*, *Revista Brasileira de Ensino de Física* **29** (2007) 645–648. 1.8.3

[5] V. I. Arnol'd, *Ordinary Differential Equations*. Springer Verlag, 1992. 1.9

[6] V. I. Arnol'd, *Geometrical Methods in the Theory of Ordinary Differential Equations*. Springer New York, 2012. 1.9

[7] L. Kantorovich, *Quantum theory of the solid state : an introduction*. Kluwer Academic Publishers, Dordrecht Boston, 2004. 1.11.1

[8] N. Ashcroft and D. Mermin, *Solid state physics*. Brooks/Cole Cengage Learning, S.l, 2003. 1.11.1

[9] C. Kittel, *Introduction to solid state physics*. Wiley, New York, 1996. 1.11.1

[10] F. Kuypers, *Klassische Mechanik*. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2016. 1.14

[11] J. Wess, *Theoretische Mechanik*. Springer-Verlag, Berlin, Heidelberg, 2008. 1.14

[12] A. Wipf, *Statistical approach to quantum field theory : an introduction*. Springer, Berlin, 2013. 1.15

[13] H. Rothe, *Lattice gauge theories : an introduction*. World Scientific, Singapore Hackensack N.J, 2012. 1.15

[14] R. Rojas, *The straight line, the catenary, the brachistochrone, the circle, and fermat*, 2014. 2.3.2

[15] K. Tapp, *Differential Geometry of Curves and Surfaces*. Springer-Verlag GmbH, 2016. 3.1.1

[16] M. Spivak, *Physics for Mathematicians, Mechanics I*. Publish or Perish, 2010. 3.2

[17] L. Schiff, *Quantum mechanics*. McGraw Hill Education (India) Private Limited, Chennai, 2017. A.2

[18] ahala (https://physics.stackexchange.com/users/34671/ahala), "How can one see that the hydrogen atom has $so(4)$ symmetry?." Physics Stack Exchange. A.2

[19] R. Gilmore, *Lie groups, physics, and geometry : an introduction for physicists, engineers and chemists*. Cambridge University Press, Cambridge, 2008. A.2

[20] M. M. (https://physics.stackexchange.com/users/14105/mark mitchison), "Relation between (super)integrability and closed orbits." Physics Stack Exchange. A.2

[21] D. M. Fradkin, *Existence of the dynamic symmetries* $\mathsf{O}(4)$ *and* $\mathsf{SU}(3)$ *for all classical central potential problems*, *Progress of Theoretical Physics* **37** (may, 1967) 798–812. A.2

[22] Y. Grandati, A. Bérard and H. Mohrbach, *On peres approach to fradkin-bacry-ruegg-souriau's perihelion vector*, *Open Physics* **9** (jan, 2011) . A.2

[23] H. Bacry, H. Ruegg and J.-M. Souriau, *Dynamical groups and spherical potentials in classical mechanics*, *Communications in Mathematical Physics* **3** (oct, 1966) 323–333. A.2

[24] J.-M. Souriau, *Structure of dynamical systems : a symplectic view of physics*. Birkhäuser, Boston, 1997, 10.1007/978-1-4612-0281-3. A.2, C.1.2

[25] M. D. Vivarelli, *The Kepler Problem S-Sphere and the Kepler Manifold*, *Meccanica* **33** (1998) 541–551. A.2

[26] C.-M. M. P. Libermann, *Symplectic Geometry and Analytical Mechanics*. Springer Netherlands, 1987. C.1.2

[27] A. Cannas da Silva, *Lectures on Symplectic Geometry*. Springer Berlin Heidelberg, free version available as well, 2008, 10.1007/978-3-540-45330-7. C.1.2

[28] H. Hofer and E. Zehnder, *Symplectic Invariants and Hamiltonian Dynamics*. Springer Basel AG, 2011. C.1.2

[29] J. Vrbik, *A novel solution to Kepler's problem*, *European Journal of Physics* **24** (May, 2003) 575. C.2

[30] W. A. Schwalm, *Lectures on selected topics in mathematical physics : elliptic functions and elliptic integrals*. Morgan & Claypool Publishers,IOP Publishing, San Rafael California (40 Oak Drive, San Rafael, CA, 94903, USA) Bristol England (Temple Circus, Temple Way, Bristol BS1 6HG, UK, 2015. C.3

[31] A. J. Brizard, *A primer on elliptic functions with applications in classical mechanics*, 0711.4064v1. C.3

[32] V. V. Prasolov and Y. Solovyev, *Elliptic functions and elliptic integrals*. American Mathematical Society, Providence, R.I, 1997. C.3