Lecture notes for Mathematical Physics 1 & 2

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Contents

1 Introduction

These lecture notes cover the "physics" part of the Mathematical Physics 1 & 2 courses at Leipzig University. We will touch on the following topics in this course: *classical mechanics* (Newtonian, Lagrangian and Hamiltonian), *Lagrangian field theory*, *gauge theories*, *Lorentzian geometry and general relativity* and *quantum mechanics*.

Since these topics all concern objects and concepts that are entirely well-defined mathematically, we can cover them with a similar style and precision as topics in mathematics. In contrast with typical physics texts on these topics, we will therefore put an emphasis on *mathematical rigour*. Roughly, this means that, we will always try to keep track of the *domains* and *codomains* are of all the maps that we consider, and we will make any underlying additional assumptions explicit. The tools and mathematical concepts that are necessary for this kind of approach will be covered in the "mathematics" part of this course.

Throughout the notes, there will be exercises, which are intended to help you interact with the text in an active manner. They are optional and are supplemented by problem sheets.

If you spot any typos or other errors, please let me know!

1.1 Some useful literature

Below you can find a list of literature that complements these lecture notes.

Classical mechanics

- Arnol'd, Vladimir Igorevich. *Mathematical methods of classical mechanics.* Vol. 60. Springer Science & Business Media, 1978.
- Thirring, Walter. *Classical mathematical physics: dynamical systems and field theories.* Springer Science & Business Media, 1997.

Lagrangian field theory

- Thirring, Walter. *Classical mathematical physics: dynamical systems and field theories.* Springer Science & Business Media, 1997.
- Frankel, Theodore. *The geometry of physics: an introduction.* Cambridge University Press, 1997.

Gauge theories

- Frankel, Theodore. *The geometry of physics: an introduction.* Cambridge University Press, 1997.
- Gutwoski, Jan. *Symmetries and Particle Physics.*, http://personal.maths.surrey.ac.uk/st/jg0033/Resources/lectnotes(master).pdf, 2007

Lorentzian geometry and general relativity

- Wald, Robert M. General relativity. University of Chicago press, 1984.
- Hawking, Stephen W., and Ellis, George F.R. *The large scale structure of space-time.* Cambridge University Press, 1973.
- Reall, Harvey. *Mathematical Tripos Part III: General relativity.* https://www.damtp.cam.ac.uk/user/hsr1000/part3_gr_lectures.pdf, 2022
- Lee, John M. *Introduction to Riemannian manifolds.* Springer, 1997.

Quantum mechanics

- Hall, Brian C. *Quantum theory for mathematicians.* Springer Publication, 2013.
- Reed, Michael, and Simon, Barry. *Methods of Modern Mathematical Physics, Volume IV: Analysis of Operators.* Academic Press, New York, 1978

2 Classical mechanics

We will refer to the vector space $\mathbb{R}^4$ as *spacetime* and we will write it as follows:

$$\mathbb{R}^4 = \mathbb{R}_t \times \mathbb{R}^3_{\mathbf{x}}.$$

The *motion of a system of* $N \in \mathbb{N}$ *particles* is the map:

$$\begin{aligned} \gamma : \mathbb{R}_t \supseteq I &\to \mathbb{R}^{3N}_{\mathbf{x}}, \\ \gamma(t) &= (\mathbf{x}_1(t), \mathbf{x}_2(t), \dots, \mathbf{x}_N(t)), \\ \mathbf{x}_i(t) &\in \mathbb{R}^3 \quad \forall 1 \leq i \leq N. \end{aligned}$$

We will make use of the following standard notation in Newtonian mechanics:

$$\begin{aligned} \dot{(\cdot)} &= \frac{d(\cdot)}{dt}, \\ \ddot{(\cdot)} &= \frac{d^2(\cdot)}{dt^2}. \end{aligned}$$

Given a vector $(t, \mathbf{x}) \in \mathbb{R} \times \mathbb{R}^3$, we will denote $x^0 = t$ and $x^i = \mathbf{x}^i$ for $i \leq i \leq 3$.

Given *masses* $m_i \in \mathbb{R}_+$ and suitably regular functions $\mathbf{F}_i : \mathbb{R}_t \times \mathbb{R}^{3N}_{\mathbf{x}} \times \mathbb{R}^{3N}_{\mathbf{x}} \to \mathbb{R}^3_{\mathbf{x}}$, with $i = 1, \dots, N$, *Newton's equations* comprise the following system of ODE (ordinary differential equations):

$$m_i \ddot{\mathbf{x}}_i(t) = \mathbf{F}_i(t, \gamma(t), \dot{\gamma}(t)) \quad 1 \leq i \leq N. \tag{2.1}$$

We interpret $\mathbf{x}_i(t)$ as the position vector of the i-th particle at time t and $\mathbf{F}_i$ as the *force* acting on the i-th particle, which is fixed by the physical setting under consideration. Equation (2.1) can then be interpreted as the statement of *Newton's Second Law* ("force equals mass times acceleration").

Newton's *Principle of Determinacy* is the statement that the motion of a system of N particles is uniquely determined by the specification of their initial positions and velocities. Continuous dependence on initial data roughly says that small changes in initial positions and velocity lead to small changes in position and velocity and later times. From the perspective of the ODE (2.1), this becomes a theorem:

Theorem 2.1 (Local well-posedness of Newton's equations)**.** *Let* $\mathbf{F}_i$ *be locally Lipschitz continuous for all* $1 \leq i \leq N$*. Given* $t_0 \in \mathbb{R}$ *and* $(\gamma_0, \gamma_1) \in \mathbb{R}^{3N} \times \mathbb{R}^{3N}$*, there exists a* $T > 0$ *and a unique* C^1 *solution* $\gamma : (t_0 - T, t_0 + T) \to \mathbb{R}^{3N}$ *to* (2.1) *satisfying*

$$(\gamma, \dot{\gamma})(t_0) = (\gamma_0, \gamma_1).$$

Furthermore, for all $\epsilon > 0$*, there exists a* $\delta > 0$*, such that if two data sets* (γ_0, γ_1) *and* $(\tilde{\gamma}_0, \tilde{\gamma}_1)$ *satisfy*

$$||(\gamma_0 - \tilde{\gamma}_0, \gamma_1 - \tilde{\gamma}_1)|| \leq \delta,$$

then for all $t \in [t_0 - \tilde{T}, t_0 + \tilde{T}]$ *with* $\tilde{T} < T$

$$||(\gamma_0 - \tilde{\gamma}_0, \gamma_1 - \tilde{\gamma}_1)(t)|| \leq \epsilon,$$

Proof. Existence and uniqueness follows directly from the Picard–Lindelöf Theorem for local existence and uniqueness of ODE, after rewriting the system as a first order system with $\mathbf{y}_i := \mathbf{x}_i$, $\mathbf{z}_i := \dot{\mathbf{x}}_i$, so $(\dot{\mathbf{y}}_i, \dot{\mathbf{z}}_i) = (\mathbf{z}_i, \mathbf{F}_i)$. Continuous dependence of data follows from a Grönwall inequality. □

For general $\mathbf{F}_i$, *global* existence and uniqueness are not guaranteed, nor is it possible to write down an expression for γ in closed form. We will, however, encounter important examples for $\mathbf{F}_i$ where we *are* able to make sense of solutions globally.

Example 2.1. *Consider a 1-particle system on* $\mathbb{R}$ *with mass* $m = 1$ *and* $F : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ *with* $F(x, v) = xv$ *and* $x(0) = x_0$, $\dot{x}(0) = \dot{x}_0$. *Then* (2.1) *gives:*

$$\ddot{x} = x\dot{x},$$

which is equivalent to

$$\dot{x} = A + x^2,$$

with $A = \dot{x}_0 - x_0^2$. *Consider initial data such that* $A = 0$.

When $\dot{x}_0 \neq 0$, *this is equivalent to the integral equation*

$$\int_{x_0}^{x(t)} y^{-2} dy = \int_0^t dt.$$

which has solutions $x(t) = \frac{1}{x_0^{-1} - t}$ *that are only well-defined for* $t < x_0^{-1}$ *or* $t > x_0^{-1}$. *Assuming additionally that the initial data satisfy* $x_0 > 0$ *therefore implies that the solutions will only exist up to* $t = x_0^{-1}$.
EXERCISE: *What can you say when the initial data satisfy* $\dot{x}_0 = 0$*?*

2.1 Principles of relativity

Newton's First Law can be roughly stated as follows: "for a mechanical system consisting of only one particle, the acceleration with respect to inertial coordinates is zero", i.e. the particle will move in a straight line and with a constant velocity. In order to make this more precise, we will introduce the notions of *Galilean transformations*.

Consider Euclidean space, which is the pair $(\mathbb{R}^n, \langle \cdot, \cdot \rangle)$, where $\langle \cdot, \cdot \rangle : \mathbb{R}^n \to \mathbb{R}^n \to \mathbb{R}$ is the Euclidean inner product: $\langle x, y \rangle = \sum_{i=1}^n x^i y^i$.

Definition 2.1. *Galilean transformations are affine maps*[1] $g = (g^0, \mathbf{g}) : \mathbb{R}_t \times \mathbb{R}^n_{\mathbf{x}} \to \mathbb{R}_t \times \mathbb{R}^n_{\mathbf{x}}$ *that preserve time intervals in* $\mathbb{R}_t$ *and norms in* $\mathbb{R}^n_{\mathbf{x}}$, *i.e. for all* $(t_1, \mathbf{x}_1), (t_2, \mathbf{x}_2) \in \mathbb{R}_t \times \mathbb{R}^n_{\mathbf{x}}$

$$|g^0(t_1, \mathbf{x}_1) - g^0(t_2, \mathbf{x}_2)| = |t_1 - t_2|,$$
$$|\mathbf{g}(t_1, \mathbf{x}_1) - \mathbf{g}(t_1, \mathbf{x}_2)| = |\mathbf{x}_1 - \mathbf{x}_2|.$$

We denote with Gal(n) *the set of all Galilean transformations on* $\mathbb{R}_t \times \mathbb{R}^n_{\mathbf{x}}$.

We will see that Galilean transformations, as well as many other symmetries that we will encounter, can naturally be describe via the notion of *groups*.

Recall,

Definition 2.2. *A group is a set* G *equipped with a binary operation* $\odot : G \times G \to G$ *that satisfies the following properties:*

1. *(Associativity.) For all* $a, b, c \in G$
$$(a \odot b) \odot c = a \odot (b \odot c).$$

2. *(Existence of an identity element.) There exists an* $e \in G$ *such that for all* $a \in G$*:*
$$e \odot a = a \odot e = a.$$

3. *(Existence of an inverse.) For all* $a \in G$, *there exists an element* $b \in G$ *such that*
$$a \odot b = b \odot a = e.$$
We denote $a^{-1} = b$.

[1] This means that $g - g(0)$ is linear.

A subgroup *of G is a subset $H \subset G$, such that $\odot(H \times H) = H$ and for all $a \in H$, $a^{-1} \in H$ (H is closed under group operations and taking the inverse).*

A group isomorphism is a bijective map between two groups $f : G \to G'$, such that for all $g, h \in G$: $f(g \odot h) = f(g) \odot f(h)$.

*A (*left*)* group action *on a set X is a map $f : G \times X \to X$ satisfying: for all $g, h \in G$ and $x \in X$*

1. $f(g \odot h, x) = f(g, f(h, x))$,
2. $f(e, x) = x$.

We will make use of the shorthand notation $g \cdot x = f(g, x)$.

EXERCISE: Show that the identity and inverse element of a group are unique.

Example 2.2. *One can easily verify that $(\mathbb{R}^n, +)$ and $(GL(\mathbb{R}^n), \cdot)$ (invertible linear maps on $\mathbb{R}^n$ with matrix multiplication) are groups. Consider*

$$O(n) = \{A \in GL(\mathbb{R}^n) \,|\, AA^T = \mathbf{1}_n\},$$
$$SO(n) = \{A \in O(n) \,|\, \det A = 1\}.$$

Then $O(n)$ is a subgroup of $GL(\mathbb{R}^n)$ (the orthogonal group) and $SO(n)$ is a subgroup of $O(n)$ (the special orthogonal group). We obtain the corresponding group actions on $\mathbb{R}_t \times \mathbb{R}^n_{\mathbf{x}}$:

1. *(Spacetime translations) Consider the group $(\mathbb{R}_t \times \mathbb{R}^n, +)$. Translations on $\mathbb{R}_t \times \mathbb{R}^n_{\mathbf{x}}$ correspond to the group action:*
$$(b^0, \mathbf{b}) \cdot (t, \mathbf{x}) = (t + b^0, \mathbf{x} + \mathbf{b}).$$
The dimension of this group (as a vector space) is $n + 1$.

2. *(Galilean boosts) Consider the group $(\mathbb{R}^n, +)$. Boosts on $\mathbb{R}_t \times \mathbb{R}^n_{\mathbf{x}}$ correspond to the group action:*
$$\mathbf{v} \cdot (t, \mathbf{x}) = (t, \mathbf{x} + t\mathbf{v}) = \begin{pmatrix} 1 & 0 \\ \mathbf{v} & 0 \end{pmatrix} \begin{pmatrix} t \\ \mathbf{x} \end{pmatrix}.$$
The dimension of this group (as a vector space) is n.

3. *(Rotations) Consider the group $(SO(n), \cdot)$. Motivated by the case $n = 3$, we refer to the group elements as "rotations". Rotations act on $\mathbb{R}_t \times \mathbb{R}^n_{\mathbf{x}}$ via the group action:*
$$R \cdot (t, \mathbf{x}) = (t, R\mathbf{x}).$$

4. *(Reflections) Consider the group $(\mathbb{Z}_2 = \{-1, 1\}, \cdot)$. Reflections through the x^i-plane on $\mathbb{R}_t \times \mathbb{R}^n_{\mathbf{x}}$ correspond to the group action:*
$$g \cdot (t, \mathbf{x}) = (t, x^1, \ldots, x^{i-1}, gx^i, x^i, \ldots, x^n).$$
Reflections in time (time reversion) correspond to the group action
$$g \cdot (t, \mathbf{x}) = (gt, \mathbf{x}).$$
EXERCISE*: Show that the dimension of $O(n)$, as a submanifold of $\mathbb{R}^{n^2}$ and $SO(n)$ is $\frac{n(n-1)}{2}$ (hint: what is the dimension of the corresponding tangent space?).*
EXERCISE*: Show that the any element of $O(n)$ is the composition of a rotation (an element of $SO(n)$) with a reflection through an x^i-plane, which corresponds to the diagonal matrix with a coefficient -1 in the ith row and all other entries equal to 1.*
EXERCISE*: Confirm that the group actions corresponding to translations, boosts, rotations and reflections are Galilean transformations.*

It turns out that translations, boosts, rotations and reflections in fact encompass *all* Galilean transformations.

Proposition 2.2. *The set of Galilean transformations* Gal(n) *can be characterized as follows:*

$$\mathrm{Gal(n)} = \left\{ (g^0, \mathbf{g}) : \mathbb{R}^{n+1} \to \mathbb{R}^{n+1} \,|\, g = T_b \circ \begin{pmatrix} \epsilon & 0 \\ \mathbf{v} & A \end{pmatrix},\ b \in \mathbb{R}^{n+1}, \mathbf{v} \in \mathbb{R}^n, A \in O(n), \epsilon \in \{1, -1\} \right\},$$

with $T_b(x) = x + b$. *Furthermore,* Gal(n) *is a group with respect to composition of maps.*

Proof. We can write

$$g(t, \mathbf{x}) = \begin{pmatrix} g^0 \\ \mathbf{g} \end{pmatrix}(t, \mathbf{x}) = \begin{pmatrix} g^0 \\ \mathbf{g} \end{pmatrix}(0, 0) + \begin{pmatrix} f^0(t, \mathbf{x}) \\ \mathbf{f}(t, \mathbf{x}) \end{pmatrix}$$

with $f^\mu(0, 0) = 0$. Hence, we can set $b = g(0, 0)$. By the assumption that g is affine, $\mathbf{f}$ must be linear in $(t, \mathbf{x})$, we can further write:

$$\mathbf{f}(t, \mathbf{x}) = A(\mathbf{x}) + t\mathbf{v},$$

for some constant $\mathbf{v} \in \mathbb{R}^n$ and a linear map $A : \mathbb{R}^n \to \mathbb{R}^n$.

We now appeal to the preservation of time intervals to conclude that:

$$|f^0(t, \mathbf{x})| = |g^0(t, \mathbf{x}) - g^0(0, 0)| = |t - 0| = |t|,$$

so $f^0(t, \mathbf{x}) = \pm t$. By continuity of f^0 (which follows from linearity), we must have that either $f^0(t, \mathbf{x}) = +t$ for all $(t, \mathbf{x})$ or $f^0(t, \mathbf{x}) = -t$ for all $(t, \mathbf{x})$.

To conclude that $A \in O(n)$, it remains to show that $A^T A = \mathbf{1}_n$. We first show that $\langle A\mathbf{x}, A\mathbf{y} \rangle = \langle \mathbf{x}, \mathbf{y} \rangle$. Indeed, by preservation of norm and linearity of A we have that

$$\langle A\mathbf{x}, A\mathbf{y} \rangle = \frac{1}{4}(|A\mathbf{x} + A\mathbf{y}|^2 - |A\mathbf{x} - A\mathbf{y}|^2) = \frac{1}{4}(|\mathbf{x} + \mathbf{y}|^2 - |\mathbf{x} - \mathbf{y}|^2) = \langle \mathbf{x}, \mathbf{y} \rangle.$$

This follows by considering basis vectors $\mathbf{e}_i$ in $\mathbb{R}^n$ and using the preservation of the Euclidean inner product to conclude that for all $i, j \in \{1, \ldots, n\}$:

$$(A^T A)^i_j = \langle \mathbf{e}_i, A^T A(\mathbf{e}_j) \rangle = \langle A(\mathbf{e}_i), A\mathbf{e}_j \rangle = \langle \mathbf{e}_i, \mathbf{e}_j \rangle = \delta^i_j,$$

with δ^i_j the Kronecker delta.

Let us now check the group property of Gal(n). First, we need to show that the composition of two Galilean transformations is a Galilean transformation.[2] Let $b_1, b_2 \in \mathbb{R}^4$, $\mathbf{v}_1, \mathbf{v}_2 \in \mathbb{R}^3$, $A, B \in O(n)$ and $\epsilon_1, \epsilon_1 \in \{-1, 1\}$. Then for any $(t, \mathbf{x}) \in \mathbb{R}^4$:

$$\begin{aligned} \left(T_{b_2} \circ \begin{pmatrix} \epsilon_2 & 0 \\ \mathbf{v}_2 & B \end{pmatrix} \right) \circ \left(T_{b_1} \circ \begin{pmatrix} \epsilon_1 & 0 \\ \mathbf{v}_1 & A \end{pmatrix} \right)(t, \mathbf{x}) &= \left(T_{b_2} \circ \begin{pmatrix} \epsilon_2 & 0 \\ \mathbf{v}_2 & B \end{pmatrix} \right) \left(\begin{pmatrix} \epsilon_1 & 0 \\ \mathbf{v}_1 & A \end{pmatrix} \begin{pmatrix} t \\ \mathbf{x} \end{pmatrix} + b_1 \right) \\ &= \begin{pmatrix} \epsilon_2\epsilon_1 & 0 \\ \epsilon_2\mathbf{v}_2 + B\mathbf{v}_1 & BA \end{pmatrix} \begin{pmatrix} t \\ \mathbf{x} \end{pmatrix} + \begin{pmatrix} \epsilon_2 & 0 \\ \mathbf{v}_2 & B \end{pmatrix} b_1 + b_2, \end{aligned}$$

Since $O(n)$ is a group, we have that $A_2 A_1 \in O(n)$, so the very right-hand side above is a Galilean transformation. Associativity follows directly from associativity of map composition. The identity element is:

$$T_e \circ \begin{pmatrix} 1 & 0 \\ 0 & \mathbf{1} \end{pmatrix}$$

Finally, by the above expression for the composition of two Galilean transformations, we can construct the inverse of $T_{b_1} \circ \begin{pmatrix} \epsilon_1 & 0 \\ \mathbf{v}_1 & A \end{pmatrix}$ as $T_{b_2} \circ \begin{pmatrix} \epsilon_2 & 0 \\ \mathbf{v}_2 & B \end{pmatrix}$, with $\epsilon_2 = \epsilon_1$, $B = A^{-1}$, $\mathbf{v}_2 = -\epsilon_2 A^{-1}\mathbf{v}_1$ and $b_2 = -\begin{pmatrix} \epsilon_2 & 0 \\ \mathbf{v}_2 & B \end{pmatrix} b_1$. □

We state without proof the folllowing proposition, which we need to interpret the Galilean group as a Lie group.

[2] This step can alternatively also be done directly from the definition of Gal(n).

Proposition 2.3. *There exists a group isomorphism between* Gal(n) *and the group*

$$\left\{ \begin{pmatrix} \epsilon & 0 & b^0 \\ \mathbf{v} & A & \mathbf{b} \\ 0 & 0 & 1 \end{pmatrix} \in GL(\mathbb{R}^{n+2}),\ b \in \mathbb{R}^{n+1}, \mathbf{v} \in \mathbb{R}^n, A \in O(n), \epsilon \in \{-1, 1\} \right\},$$

so Gal(n) *in a matrix Lie group (a closed subset of* $GL(\mathbb{R}^{n+2})$*).*

The dimension of Gal(n) *is* $\frac{1}{2}n(n-1) + (n+1) + n$*.*

Definition 2.3. *Let* $\Phi : \mathbb{R}_t \times \mathbb{R}^n_{\mathbf{x}} \supset I \times U \to J \times V \subset \mathbb{R}_t \times \mathbb{R}^n_{\mathbf{x}}$ *determine a coordinate chart* $\{\Phi^\alpha\}$*, with* I, J, U, V *open subsets, i.e.* Φ *is a smooth diffeomorphism between* $I \times U$ *and* $J \times V$*. Then* $\{\Phi^\alpha\}$ *is an* inertial coordinate chart*, an* inertial frame *or a* Galilean coordinate transformation *if* $U = V = \mathbb{R}^n_{\mathbf{x}}$*,* $I = J = \mathbb{R}_t$ *and* $\Phi \in \text{Gal}(n)$*.*

We can represent the path of N particles $t \mapsto \mathbf{x}_i(t)$, $1 \leq i \leq N$, with respect to the coordinate chart $\{\Phi^\alpha\}$. We write $(t', \mathbf{y}) = (\Phi^0, \Phi^1, \Phi^2, \Phi^3)$ and consider the paths $t \mapsto \mathbf{y}(t, \mathbf{x}_i(t))$ in $\mathbb{R}^3$. We reparametrize this path as follows: in slight abuse of notation, we write $t'(t) = t'(t, \mathbf{x}_i(t))$ and denote the corresponding inverse as $t(t')$. Then we define $\mathbf{y}_i(t') := \mathbf{y}(t(t'), \mathbf{x}_i(t(t')))$. If $t' = \pm t + s$, then $t(t') = \pm(t' - s)$, so $\mathbf{y}_i(t') := \mathbf{y}(\pm(t' - s), \mathbf{x}_i(\pm(t' - s)))$

Definition 2.4. *We say the forces appearing in the equations* (2.1) *satisfy the* principle of Galilean relativity *if for any Galilean coordinate transformation* $\Phi = (t', \mathbf{y}) : \mathbb{R}_t \times \mathbb{R}^3_{\mathbf{x}} \to \mathbb{R}_t \times \mathbb{R}^3_{\mathbf{x}}$ *and any solution* $t \mapsto \mathbf{x}_i(t)$ *of* (2.1)*:*

$$m_i \frac{d^2 \mathbf{y}_i}{dt'^2}(t') = \mathbf{F}_i \left(t', \mathbf{y}_1(t'), \ldots, \mathbf{y}_N(t'), \frac{d\mathbf{y}_1}{dt'}(t'), \ldots, \frac{d\mathbf{y}_N}{dt'}(t') \right).$$

We say in this case that (2.1) *are* invariant *under Galilean transformations. We can similarly consider forces that are invariant under a subgroup of Galilean transformations (e.g., translations, rotatations).*

The principle of Galilean relativity can be interpreted as saying that physical laws remain the same in different inertial frames. We can interpret this as follows: two observers will agree on the motion described by particles determined by forces satisfying the principle of Galilean relativity, with a prescribed initial position and velocity, if:

- the observers have a constant relative velocity,
- the observers are rotated with respect to each other,
- one observer looks at the particles through a mirror ("through the looking glass"),
- one observer moves backwards in time compared to the other.

Observers will, for example, not agree if they experience a non-trivial relative acceleration or if they rotate at a non-zero relative angular velocity.

Classical mechanics is predicated on the existence of a preferred class of inertial coordinates (related by Galilean transformations), with respect to which forces should be defined and Newton's equation is formulated. In practice, one treats the frame associated to the earth, the sun or the stars as an "approximate" inertial frame, depending on the scale of the system under consideration. All coordinate charts related to this frame via Galilean transformations make up the relevant class of inertial frames.

Proposition 2.4. *Let* $\mathbf{F}_i : \mathbb{R}_t \times \mathbb{R}^{3N} \times \mathbb{R}^{3N} \to \mathbb{R}^3$*,* $i = 1, \ldots, N$ *be forces that are invariant under time translations. Then* $\mathbf{F}_i(t, \cdot) = \mathbf{F}_i(0, \cdot)$ *for all* $t \in \mathbb{R}$ *and* $i = 1, \ldots, N$*.*

Proof. Consider the coordinate chart $(t', \mathbf{y}) = (t + s, \mathbf{x})$. Then, by the invariance property of $\mathbf{F}_i$:

$$\begin{aligned} \mathbf{F}_i(t + s, \mathbf{x}_1(t), \ldots, \mathbf{x}_N(t), \dot{\mathbf{x}}_1(t), \ldots, \dot{\mathbf{x}}_N(t)) &= m \frac{d^2 \mathbf{y}_i}{dt'^2}(t') \\ &= m \frac{d^2 \mathbf{x}_i}{dt^2}(t) = \mathbf{F}_i(t, \mathbf{x}_1(t), \ldots, \mathbf{x}_N(t), \dot{\mathbf{x}}_1(t), \ldots, \dot{\mathbf{x}}_N(t)). \end{aligned}$$

We can take $t = 0$ and choose $\gamma(0)$, $\dot{\gamma}(0)$ arbitrary, to conclude that $\mathbf{F}_i(s, \cdot) = \mathbf{F}_i(0, \cdot)$ for all $s \in \mathbb{R}$. □

Proposition 2.5 (Newton's First Law)**.** *If* (2.1) *with* $N = 1$ *satisfies the principle of Galilean relativity, then* $\ddot{\mathbf{x}} \equiv 0$*, i.e. the particle moves in a straight line at constant velocity in an inertial frame.*

Proof. Under spacetime translations which preserve the time direction together with boosts, $(t', \mathbf{y}) = (t + s, \mathbf{x} + \mathbf{b} + t\mathbf{v})$, we have that $\frac{d\mathbf{y}}{dt'}(t') = \frac{d\mathbf{x}}{dt}(t) + \mathbf{v}$ and therefore $\frac{d^2\mathbf{y}}{dt'^2}(t') = \frac{d^2\mathbf{x}}{dt^2}(t)$. Hence,

$$\mathbf{F}(t + s, \mathbf{x}(t) + \mathbf{b} + t\mathbf{v}, \dot{\mathbf{x}}(t) + \mathbf{v}) = \mathbf{F}\left(t', \mathbf{y}(t'), \frac{d\mathbf{y}}{dt}(t')\right) = m\frac{d^2\mathbf{y}}{dt'^2}(t') = m\frac{d^2\mathbf{x}}{dt^2}(t) = \mathbf{F}(t, \mathbf{x}(t), \dot{\mathbf{x}}(t)).$$

By Proposition 2.4, we already know that $\mathbf{F}$ must be independent of t. Now, we take $s = 0$ and $\mathbf{v} = 0$, so that

$$\mathbf{F}(t, \mathbf{x}(t) + \mathbf{b}, \dot{\mathbf{x}}(t)) = \mathbf{F}(t, \mathbf{x}(t), \dot{\mathbf{x}}(t)),$$

from which it follows that $\mathbf{F}$ must also be independent of $\mathbf{x}$. Setting $s = 0$ and $\mathbf{b} = 0$, similarly gives independence of $\mathbf{v}$. We therefore conclude that $\mathbf{F}(t, \mathbf{x}, \dot{\mathbf{x}}) = \mathbf{F}_0$ must be a constant vector.

Finally, consider an arbitrary rotation $R \in SO(3)$. Then $\frac{d\mathbf{y}_i}{dt'}(t') = R\frac{d\mathbf{x}_i}{dt}$. Hence, $\mathbf{F}_0 = \mathbf{F}(t, R\mathbf{x}, R\dot{\mathbf{x}}) = R\mathbf{F}(t, \mathbf{x}, \dot{\mathbf{x}}) = R\mathbf{F}_0$. Since the only vector that is invariant under all rotations in the zero vector, we conclude that $\mathbf{F}_0 = 0$. □

Proposition 2.6. *If* (2.1) *with general* $N \in \mathbb{N}$ *satisfies the principle of Galilean relativity, then there exists maps* $\mathbf{f}_i : \mathbb{R}^{3(\frac{1}{2}N(N-1))} \to \mathbb{R}^3$ *such that*

$$\mathbf{F}_i(t, \mathbf{x}_1, \ldots, \mathbf{x}_N, \dot{\mathbf{x}}_1, \ldots, \dot{\mathbf{x}}_N) = \mathbf{f}_i(\mathbf{X}, \dot{\mathbf{X}}),$$

with $\mathbf{X}$ *and* $\dot{\mathbf{X}}$ *antisymmetric* $N \times N$ *matrices whose components are the following vectors in* $\mathbb{R}^3$*:* $\mathbf{X}_{ij} = \mathbf{x}_i - \mathbf{x}_j$ *and* $\dot{\mathbf{X}}_{ij} = \dot{\mathbf{x}}_i - \dot{\mathbf{x}}_j$*, respectively.*

For any $A \in O(3)$

$$A\mathbf{f}_i(\mathbf{X}, \dot{\mathbf{X}}) = \mathbf{f}_i(A \cdot \mathbf{X}, A \cdot \dot{\mathbf{X}}),$$

where $(A \cdot \mathbf{X})_{ij} := A(\mathbf{x}_i - \mathbf{x}_j)$ *and* $A \cdot \dot{\mathbf{X}} := A(\dot{\mathbf{x}}_i - \dot{\mathbf{x}}_j)$*.*

If we assume moreover that (2.1) *is invariant under a permutation of the particles (i.e. the particles are indistinguishable), then* $\mathbf{f}_i$ *can be redefined as as a function depending only on the* N *vectors:* $\mathbf{x}_i - \mathbf{x}_j$*, with* $j = 1, \ldots, N$*.*

Proof. By Proposition 2.4, $\mathbf{F}_i$ must be time-independent. By invariance under translations in $\mathbb{R}^3$, $\mathbf{F}_i$ must depend only on relative spatial coordinates $\mathbf{x}_j - \mathbf{x}_k$. By invariance under boosts, $\mathbf{F}_i$ must also only depend on relative velocities $\dot{\mathbf{x}}_j - \dot{\mathbf{x}}_k$. Finally, we appeal to invariance under $O(3)$ to conclude that for all $A \in O(3)$:

$$A\mathbf{f}_i(\mathbf{X}, \dot{\mathbf{X}}) = \frac{d^2(A\mathbf{x})_i}{dt^2}(t) = \mathbf{F}_i(t, A\mathbf{x}_1(t), \ldots, A\mathbf{x}_N(t), A\dot{\mathbf{x}}_1(t), \ldots, A\dot{\mathbf{x}}_N(t)) = \mathbf{f}_i(A \cdot \mathbf{X}, A \cdot \dot{\mathbf{X}}).$$

Finally, suppose $\mathbf{F}_i$ is invariant under a permutation of the particles, i.e. under an exchange of $\mathbf{x}_j$ and $\mathbf{x}_k$ for $j \neq k$ and $j, k \neq i$. Then $\mathbf{F}_i$ can only depend on relative distances involving $\mathbf{x}_i$. □

Remark 2.1. *Examples of physical theories satisfying the principle of Galilean relativity: Newtonian gravity, (non-relativistic) Euler's equations of fluid mechanics. Counter-example: Maxwell equations. Navier–Stokes equations are not invariant under time reversal, but they are invariant under all other Galilean transformations.*

We define the Lorentzian inner product of $x, y \in \mathbb{R}^{n+1}$ as the following, symmetric bilinear and non-degenerate form:

$$m(x, y) = -x^0 y^0 + \sum_{i=1}^{n} x^i y^i.$$

Note that $m(x, x)$ is <u>not</u> positive definite, so $\sqrt{m(x, x)}$ does not define a norm.

Definition 2.5. *Poincaré transformations are affine maps $g : \mathbb{R}^{n+1} \to \mathbb{R}^{n+1}$, with $n \geq 1$, that preserve Lorentzian length, i.e.*

$$m(g(x) - g(y), g(x) - g(y)) = m(x - y, x - y) \quad \forall x, y \in \mathbb{R}^{n+1}.$$

We denote the set of of Poincaré transformations in $\mathbb{R}^{n+1}$ by $P(n; 1)$.

We give a little bit of motivation for the definition of m. By the requirement that our "inertial frames" should have the property that the speed of light c stays constant. Indeed, let $(t_1, \mathbf{x}_1) \in \mathbb{R}^{n+1}$ denote the spacetime event of emission of a "light signal" (for the purposes of this argument, this is a particle travelling at speed c) and $(t_2, \mathbf{x}_2) \in \mathbb{R}^{n+1}$ the spacetime event of absorption of the light signal. Then the spatial distance between these two spacetime events is $\sqrt{\sum_{i=1}(x_1^i - x_2^i)^2}$, but it should also be $c(t_2 - t_1)$ (speed $\times$ time). Hence:

$$-c^2(t_2 - t_1)^2 + \sum_{i=1}(x_1^i - x_2^i)^2 = 0.$$

If we describe the same event with respect to different spacetime coordinates $(t', \mathbf{y})$, we should similarly have that:

$$-c^2(t_2 - t_1)^2 + \sum_{i=1}(x_1^i - x_2^i)^2 = 0 = -c^2(t_2' - t_1')^2 + \sum_{i=1}(y_1^i - y_2^i)^2.$$

Hence, the Lorentzian length is preserved for spacetime intervals $x_1 - x_2$, which satisfy $m(x_1 - x_1, x_1 - x_2) = 0$. One can further argue that the Lorentzian length should also be preserved even if $m(x_1 - x_1, x_1 - x_2) \neq 0$, but we will omit this part of the argument.

Example 2.3. *The following group actions on $\mathbb{R}^{n+1}$ are examples of Poincaré transformations:*

1. *(Translations) The translation group $(\mathbb{R}^{n+1}, +)$ with group action*

$$b \cdot x = x + b.$$

2. *(Rotations and reflections in space) The group $(O(n), \cdot)$ with group action*

$$A \cdot x = (x^0, A\mathbf{x}).$$

Let $\mathbf{n}$ be a unit norm vector, $v \in [0, 1)$ and $\gamma = \frac{1}{\sqrt{1-v^2}}$. Then following map is also a Poincaré transformation:

$$x \mapsto (\gamma(x^0 - v\mathbf{n} \cdot \mathbf{x}), \mathbf{x}_\perp + \gamma(\mathbf{x}_{||} - vx^0\mathbf{n})),$$

where $\mathbf{x}_{||} = \langle \mathbf{x}, \mathbf{n} \rangle \mathbf{n}$ and $\mathbf{x}_\perp = \mathbf{x} - \mathbf{x}_{||}$. This map is called a Lorentz boost *in the $\mathbf{n}$–direction.*
EXERCISE: *Show that boosts do not correspond to group actions, by considering a composition of two boosts.*

We say a physical theory satisfies the *principle of special relativity* if it is "invariant under Poincaré transformations". That is to say, the laws of physics should remain unchanged when passing to a different inertial frame, which is related to the original coordinates via a Poincaré transformation. We will explore what this means precisely in the context of field theories.

EXERCISE: Show that the force term on the right-hand side of Newton's equations of gravity changes when we perform a coordinate change corresponding to a Poincaré transformation.

We will later see that Maxwell's equations of electromagnetism *are* invariant under Poincaré transformations.

Proposition 2.7. *We can write:*

$$P(n; 1) = \left\{ g : \mathbb{R}^{n+1} \to \mathbb{R}^{n+1} \,|\, g = T_b \circ \Lambda, \ , b \in \mathbb{R}^{n+1}, \Lambda \in O(n; 1) \right\},$$

where

$$O(n; 1) = \{\Lambda \in GL(\mathbb{R}^{n+1}) \,|\, m(\Lambda x, \Lambda y) = m(x, y)\}$$

is the subset of Lorentz transformations.

Furthermore, for any $\Lambda \in O(n;1)$, there exist $A \in O(n)$, $R \in SO(n)$, $\psi \in \mathbb{R}$ and $\epsilon \in \{-1,1\}$, such that

$$\Lambda = \begin{pmatrix} \epsilon & 0 \\ 0 & A \end{pmatrix} L_\psi \begin{pmatrix} 1 & 0 \\ 0 & R \end{pmatrix},$$

with

$$L_\psi = \begin{pmatrix} \cosh\psi & 0 & \dots & 0 & \sinh\psi \\ 0 & & & & 0 \\ \vdots & & \mathbf{1}_{n-1} & & \vdots \\ 0 & & & & 0 \\ \sinh\psi & 0 & \dots & 0 & \cosh\psi \end{pmatrix}.$$

a Lorentz boost in the direction of the nth coordinate axis. *The set $P(n;1)$ forms a group under function composition.*

Proof. Problem Sheet 3. □

Remark 2.2. *We can express*

$$\cosh\psi = \frac{1}{\sqrt{1-v^2}},$$
$$\sinh\psi = \frac{v}{\sqrt{1-v^2}},$$

with $v^2 < 1$ to put L_ψ in the more familiar form of a boost in the x^n-direction.

Proposition 2.8. *There exists a group isomorphism between $P(n;1)$ and*

$$\left\{ \begin{pmatrix} A & b \\ 0 & 1 \end{pmatrix} \in GL(\mathbb{R}^{n+2}),\ b \in \mathbb{R}^{n+1}, A \in O(n;1) \right\},$$

so $P(n;1)$ in a matrix Lie group.

Proof. Exercise. □

Remark 2.3. *Consider the subgroup $O(n;1)$ of Lorentz transformations.*

- *By restricting to $\Lambda \in O(n;1)$ with $\det\Lambda = 1$, we obtain the subgroup $SO(n;1)$ called the* proper Lorentz group.
- *By restricting to $\Lambda \in O(n;1)$ with $\Lambda_{00} > 0$, we obtain the* orthochonous Lorentz group $O(n;1)^+$.
- *By restricting to $\Lambda \in SO(n;1)$ with $\Lambda_{00} > 0$, we obtain the* proper, orthochronous Lorentz group $SO(n;1)^+$.

When viewed as a topological space, $O(n;1)$ has four connected components and the component $SO(n;1)^+$ is one of these, namely the one that contains the identity element.

2.2 Conservative forces

We will now consider (2.1) with some additional restrictions. We make the following assumption: for all $1 \le i \le N$

$$\mathbf{F}_i(t, \mathbf{x}_1, \dots, \mathbf{x}_N, \mathbf{v}_1, \dots, \mathbf{v}_N) = -\nabla_{\mathbf{x}_i} U(\mathbf{x}_1, \dots, \mathbf{x}_N), \tag{2.2}$$

for some C^2 function $U : \mathbb{R}^{3N} \to \mathbb{R}$, which we call the *potential*. Here $\nabla_{\mathbf{x}_i}$ denotes the gradient with respect to $\mathbf{x}_i$. We call $\mathbf{F}_i$ satisfying (2.2) *conservative forces*. Note that, in particular, we are assuming that $\mathbf{F}_i$ are independent of t and the velocity variables $\mathbf{v}_j$.

An equivalent way of characterizing conservative forces in the $N = 1$ case is as C^1 functions with the form $\mathbf{F}_i(\mathbf{x})$ and additionally being path independent, i.e. for any piecewise C^1 closed loop $\mathbb{S}^1 \ni t \mapsto \mathbf{x}$

$$\int_{\mathbb{S}^1} \mathbf{F}_i(\mathbf{x}(t)) \cdot \dot{\mathbf{x}}(t)\, dt = 0.$$

Yet another equivalent way of characterizing the conservative property of $\mathbf{F}(\mathbf{x})$ in the $N = 1$ case is:

$$\nabla \times \mathbf{F} \equiv 0.$$

The characteristic and very useful property of solutions to Newton's equations with conservative forces is that they admit a conserved energy. We define the *energy associated to* $\gamma : I \to \mathbb{R}^{3N}$ as follows:

$$E_\gamma(t) = \sum_{i=1}^{N} \frac{1}{2} m_i |\dot{\mathbf{x}}_i|^2(t) + U(\mathbf{x}_1(t), \dots, \mathbf{x}_N(t)).$$

The energy has the property that it is conserved in time.

Proposition 2.9. *Let $\gamma : I \to \mathbb{R}^{3N}$ be a solution to (2.1) with forces $\mathbf{F}_i$ satisfying (2.2). Then $\frac{d}{dt} E_\gamma(t) = 0$.*

Proof. By the chain rule, we have that

$$\begin{aligned}\frac{d}{dt} E_\gamma(t) &= \sum_{i=1}^{N} \frac{1}{2} m_i \frac{d}{dt} |\dot{\mathbf{x}}_i|^2(t) + \frac{d}{dt} U(\mathbf{x}_1(t), \dots, \mathbf{x}_N(t)) \\ &= \sum_{i=1}^{N} m_i \langle \ddot{\mathbf{x}}_i, \dot{\mathbf{x}}_i \rangle(t) + \sum_{i=1}^{N} \langle \nabla_{\mathbf{x}_i} U(\mathbf{x}_1(t), \dots, \mathbf{x}_N(t)), \dot{\mathbf{x}}_i \rangle \\ &= \sum_{i=1}^{N} \langle m_i \ddot{\mathbf{x}}_i(t) + \nabla_{\mathbf{x}_i} U(\mathbf{x}_1(t), \dots, \mathbf{x}_N(t)), \dot{\mathbf{x}}_i \rangle = 0. \quad \square\end{aligned}$$

Proposition 2.10. *Let $\mathbf{F} : \mathbb{R}^3_{\mathbf{x}} \setminus \{0\} \to \mathbb{R}^3$ be C^1 and invariant with respect to $SO(3)$, i.e. $\mathbf{F}$ is a central force that needs not be defined at the origin. Then $\mathbf{F}$ is conservative.*

Proof. We can decompose $\mathbb{R}^3 \cong T_{\mathbf{x}}\mathbb{R}^3 \ni \mathbf{F}(\mathbf{x}) = F^r(\mathbf{x})\mathbf{e}_r(\mathbf{x}) + F^\theta(\mathbf{x})\mathbf{e}_\theta(\mathbf{x}) + F^\varphi(\mathbf{x})\mathbf{e}_\varphi(\mathbf{x})$, with $\{\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{e}_\varphi\}$ an orthonormal basis of vector fields such that the vector field $\mathbf{e}_r$ is defined as follows $\mathbf{e}_r(\mathbf{x}) = \frac{\mathbf{x}}{|\mathbf{x}|}$, $\mathbf{e}_\theta$ points in the direction of increasing θ angle and $\mathbf{e}_\varphi$ points in the direction of increasing φ angle, with respect to standard spherical coordinates (r, θ, φ).

By assumption, $\mathbf{F}$ is invariant under rotations $R \in SO(3)$, so $R\mathbf{F}(\mathbf{x}) = \mathbf{F}(R\mathbf{x})$. By taking R to be a 180° rotation around the axis through $\mathbf{e}_r(\mathbf{x})$ (so, in particular $R\mathbf{e}_r(\mathbf{x}) = \mathbf{e}_r(\mathbf{x})$ and $R\mathbf{x} = \mathbf{x}$), we obtain

$$F^r(\mathbf{x})\mathbf{e}_r(\mathbf{x}) - F^\theta(\mathbf{x})\mathbf{e}_\theta(\mathbf{x}) - F^\varphi(\mathbf{x})\mathbf{e}_\varphi(\mathbf{x}) = R\mathbf{F}(\mathbf{x}) = \mathbf{F}(R\mathbf{x}) = \mathbf{F}(\mathbf{x}) = F^r(\mathbf{x})\mathbf{e}_r(\mathbf{x}) + F^\theta(\mathbf{x})\mathbf{e}_\theta(\mathbf{x}) + F^\varphi(\mathbf{x})\mathbf{e}_\varphi(\mathbf{x}).$$

Hence $F^\theta = F^\varphi = 0$. Now let R be a general rotation, then $F^r(\mathbf{x})R\mathbf{e}_r(\mathbf{x}) = F^r(R\mathbf{x})\mathbf{e}_r(R\mathbf{x}) = F^r(R\mathbf{x})R\mathbf{e}_r(\mathbf{x})$, so $F^r(R\mathbf{x}) = F^r(\mathbf{x})$. In spherical coordinates (r, θ, φ), this means that we can write:

$$\mathbf{F}(\mathbf{x}) = F^r(r)\mathbf{e}_r(\mathbf{x}).$$

Now, for arbitrary $r_0 > 0$, define $U : \mathbb{R}^3_{\mathbf{x}} \setminus \{0\} \to \mathbb{R}$ as follows with respect to spherical coordinates

$$U(r, \theta, \varphi) = -\int_{r_0}^{r} F^r(r')\, dr'. \qquad \square$$

Example 2.4 (Particle in one dimension)**.** *Consider Newton's equation on $I \subset \mathbb{R}$ with $F(t, x, \dot{x}) = F(x)$. Then we can write*

$$m\ddot{x}(t) = F(x(t)) = -U'(x(t)),$$

with $U(x) = -\int_{x_0}^{x} F(x')\, dx'$, with $x_0 \in I$ arbitrary.

Example 2.5 (Newton's theory of gravity)**.**

$$m_i\ddot{\mathbf{x}}_i = -\nabla_{\mathbf{x}_i} U(\mathbf{x}_1, \dots, \mathbf{x}_N),$$
$$U(\mathbf{x}_1, \dots, \mathbf{x}_N) = -\sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{m_i m_j}{|\mathbf{x}_i - \mathbf{x}_j|}.$$

Let $t \mapsto \mathbf{x}(t)$ denote a C^2 path in $\{z = 0\} \subset \mathbb{R}^3$. We denote $r(t) = |\mathbf{x}(t)|$ and $\mathbf{e}_r(\mathbf{x}) = \frac{\mathbf{x}}{r}$. In polar coordinates, we can write $\mathbf{e}_r(\mathbf{x}) = (\cos\varphi, \sin\varphi, 0)^T$. We denote with $\mathbf{e}_\varphi(\mathbf{x})$ the corresponding orthogonal, unit norm vector field that points in the direction of increasing φ. Then $\mathbf{e}_\varphi(\mathbf{x}) = (-\sin\varphi, \cos\varphi, 0)^T$. Let $\mathbf{e}_z$ denote the constant unit norm vector field pointing in the z-direction in $\mathbb{R}^3$. Then $\{\mathbf{e}_r(\mathbf{x}), \mathbf{e}_\varphi(\mathbf{x}), \mathbf{e}_z(\mathbf{x})\}$ form an orthonormal basis for $T_{\mathbf{x}}\mathbb{R}^3$, in particular along the path $t \mapsto \mathbf{x}(t)$.

Note that

$$\partial_r \mathbf{e}_r(\mathbf{x}) = \partial_r \mathbf{e}_\varphi(\mathbf{x}) = 0,\ \partial_\varphi \mathbf{e}_r(\mathbf{x}) = \mathbf{e}_\varphi(\mathbf{x}) \text{ and } \partial_\varphi \mathbf{e}_\varphi(\mathbf{x}) = -\mathbf{e}_r(\mathbf{x}).$$

By construction, we have that $\mathbf{x}(t) = r(t)\mathbf{e}_r(\mathbf{x}(t))$, so by the chain rule:

$$\begin{aligned}\dot{\mathbf{x}}(t) &= \dot{r}(t)\mathbf{e}_r(\mathbf{x}(t)) + r(t)\dot{\mathbf{e}}_r(\mathbf{x}(t)) \\ &= \dot{r}(t)\mathbf{e}_r(\mathbf{x}(t)) + r(t)\dot{\varphi}\partial_\varphi \mathbf{e}_r(\mathbf{x}(t)) \\ &= \dot{r}(t)\mathbf{e}_r(\mathbf{x}(t)) + r(t)\dot{\varphi}\mathbf{e}_\varphi(\mathbf{x}(t)).\end{aligned} \tag{2.3}$$

We can express the angular momentum $\mathbf{L} = \mathbf{x} \times m\dot{\mathbf{x}}$ as follows using (2.3):

$$\mathbf{L} = \mathbf{x} \times m\dot{\mathbf{x}} = mr^2\dot{\varphi}\mathbf{e}_r \times \mathbf{e}_\varphi = mr^2\dot{\varphi}\mathbf{e}_z. \tag{2.4}$$

Proposition 2.11 (Central force in 2 dimensions)**.** *Consider Newton's equation in $\mathbb{R}^3$ with a central force that is restricted to the plane $\{z = 0\}$:*

$$m\ddot{\mathbf{x}} = \mathbf{F}(0, x^1, x^2) = -\nabla U(0, x^1, x^2).$$

Then $r(t)$ satisfies Newton's equation on $\mathbb{R}_+$ with respect to a force corresponding to the potential

$$V(r) = U(r) + \frac{L^2}{2mr^2},$$

with $L = |\mathbf{L}|$ and $\mathbf{L}$ conserved in time. The potential V is called the effective potential*.*

Proof. Note that

$$\ddot{\mathbf{x}} = \frac{d}{dt}(\dot{r}\mathbf{e}_r + r\dot{\varphi}\mathbf{e}_\varphi) = (\ddot{r} - r\dot{\varphi}^2)\mathbf{e}_r + (2\dot{r}\dot{\varphi} + r\ddot{\varphi})\mathbf{e}_\varphi.$$

Using that $\mathbf{F}$ is central, we have that with respect to polar coordinates (r, φ), U depends only on r and $\mathbf{F} = -\partial_r U \mathbf{e}_r$, so

$$\begin{aligned} m\ddot{r} - mr\dot{\varphi}^2 &= -\partial_r U \\ 2m\dot{r}\dot{\varphi} + mr\ddot{\varphi} &= 0.\end{aligned}$$

Note that the second equation is equivalent to $\frac{d}{dt}(mr^2\dot{\varphi}) = 0$. Since $\mathbf{L} = mr^2\dot{\varphi}\mathbf{e}_z$, this implies conservation of angular momentum $\mathbf{L}(\mathbf{x}(t))$ in time. We therefore have that $\dot{\varphi} = \frac{\pm L}{mr^2}$. Filling this in, we obtain:

$$m\ddot{r} = -\partial_r U(r, \varphi) + \frac{L^2}{mr^3} = -V'(r). \qquad \square$$

2.3 Calculus of variations

We consider maps of the form:

$$\mathcal{S} : C^1([a,b];\mathbb{R}^n) \to \mathbb{R},$$

where $C^1([a,b];\mathbb{R}^n)$ is the space of continuous functions from the interval $[a,b]$ to $\mathbb{R}^n$. Maps of the form $X \to \mathbb{R}$ or $X \to \mathbb{C}$, with X an appropriate function space, are called *functionals*.

To do calculus of variations, we need to study how $\mathcal{S}$ changes when vary γ, while keeping its endpoints fixed, i.e. we consider

$$\mathcal{S}(\gamma + sh),$$

with $s \in \mathbb{R}$ and $h \in C_0^1((a,b);\mathbb{R}^n)$ (h is C^1 and compactly supported on (a,b)).

In this section, we will restrict to $\mathcal{S}$ of the following form:

$$\mathcal{S}(\gamma) = \int_a^b \mathcal{L}(t,\gamma(t),\dot\gamma(t))\,dt, \tag{2.5}$$

with $\mathcal{L} \in C^2(\mathbb{R}_t \times \mathbb{R}^n_x \times \mathbb{R}^n_v)$, i.e. $\mathcal{L}$ is continuously differentiable. We will refer to such a functional as an *action* on $[a,b]$ and the functions $\mathcal{L}$ as *Lagrangians*.

We denote the partial derivative of $\mathcal{L}$ with respect to the first n variables with $\partial_{x^i}\mathcal{L}$, with respect to next n variables with $\partial_{v^i}\mathcal{L}$ and with respect to the third variable with $\partial_t\mathcal{L}$. When considering a path $\gamma : [a,b] \to \mathbb{R}^n$ with derivative $\dot\gamma$, we can apply the chain rule to determine derivatives of the composition $\widetilde{\mathcal{L}} = \mathcal{L} \circ (\mathrm{id}, \gamma, \dot\gamma)$. For example,

$$\frac{d}{dt}\widetilde{\mathcal{L}}(t) = \sum_{i=1}^n \partial_{x^i}\mathcal{L}(t,\gamma(t),\dot\gamma(t))\dot\gamma^i(t) + \partial_{v^i}\mathcal{L}(t,\gamma(t),\dot\gamma(t))\ddot\gamma^i(t) + \partial_t\mathcal{L}(t,\gamma(t),\dot\gamma(t)).$$

Theorem 2.12. *Let $\mathcal{S}$ satisfy (2.5) and let $h \in C_0^1((a,b);\mathbb{R}^n)$. Then*

$$\frac{d}{ds}\Big|_{s=0}\mathcal{S}(\gamma+sh) = \int_a^b \left[\frac{\partial\mathcal{L}}{\partial x^i} - \frac{d}{dt}\frac{\partial\mathcal{L}}{\partial v^i}\right](t,\gamma(t),\dot\gamma(t))h^i\,dt.$$

Here we use the Einstein summation convention*: we omit the sum symbol "$\Sigma_{i=1}^n$" when there are repeated indices, i.e. $v^iw_i = \sum_{i=1}^n v^iw_i$.*

Proof. We have that:

$$\begin{aligned}
\frac{d}{ds}\Big|_{s=0}\mathcal{S}(\gamma+sh) &= \lim_{s\to0}\frac{1}{s}\int_a^b \mathcal{L}(t,\gamma(t)+sh(t),\dot\gamma(t)+s\dot h(t)) - \mathcal{L}(t,\gamma(t),\dot\gamma(t))\,dt \\
&= \int_a^b \frac{\partial\mathcal{L}}{\partial x^i}(t,\gamma(t),\dot\gamma(t))h^i + \frac{\partial\mathcal{L}}{\partial v^i}(t,\gamma(t),\dot\gamma(t))\dot h^i\,dt \\
&= \int_a^b \frac{\partial\mathcal{L}}{\partial x^i}(t,\gamma(t),\dot\gamma(t))h^i - \frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial v^i}\right)(t,\gamma(t),\dot\gamma(t))\dot h^i\,dt + \cancel{\frac{\partial\mathcal{L}}{\partial v^i}(t,\gamma(t),\dot\gamma(t))h^i(t)\Big|_{t=a}^{t=b}}
\end{aligned}$$

□

In the literature, you will sometimes encounter the notation "$\delta\mathcal{S}$" or "$\frac{\delta\mathcal{S}}{\delta h}$" for $\frac{d}{ds}|_{s=0}\mathcal{S}(\gamma+sh)$.

Definition 2.6. *An* extremal *is a curve $\gamma \in C^1([a,b];\mathbb{R}^n)$ such that*

$$\frac{d}{ds}\Big|_{s=0}\mathcal{S}(\gamma+sh) = 0$$

for all $h \in C_0^1((a,b);\mathbb{R}^n)$.

An extremal curve may also minimize the functional, i.e. $\mathcal{S}(\delta) \geq \mathcal{S}(\gamma)$, for all $\delta \in C^1([a,b]\ \mathbb{R}^n)$, but this need not always be the case. A curve γ is a *local minimum* if

$$\frac{d^2}{ds^2}\Big|_{s=0}\mathcal{S}(\gamma+sh) > 0$$

for all $h \in C_0^2((a,b);\mathbb{R}^n)$.

Lemma 2.13. *Let $f \in C^0([a,b];\mathbb{R})$, such that for every $\phi \in C^\infty([a,b];\mathbb{R})$, with $\phi(a) = \phi(b) = 0$:*

$$\int_a^b f(t)\phi(t)\,dt = 0.$$

Then $f \equiv 0$.

Proof. We will prove the lemma by contradiction. Suppose there exists a $t_0 \in [a,b]$ such that $c := f(t_0) \neq 0$. Without loss of generality, assume that $c > 0$ (otherwise, just consider $-f$ instead of f). Then, by continuity of f, there exists a $\delta > 0$, such that

$$f(t) > \frac{c}{2}$$

in $(t_0 - \delta, t_0 + \delta)$.

To reach a contradiction, will will construct a ϕ that vanishes in $[a,b] \setminus (t_0 - \delta, t_0 + \delta)$ and is positive on $(t_0 - \delta, t_0 + \delta)$.

We consider first the bump function or mollifier $\eta \in C^\infty(\mathbb{R})$:

$$\eta(x) = \begin{cases} e^{-\frac{1}{1-|x|^2}} & \text{if } |x| < 1, \\ 0 & \text{if } |x| \geq 1, \end{cases}$$

Let $\phi(t) = \eta(\frac{2}{\delta}(t - t_0))$. Then, by continuity, there exists an $0 < \epsilon < \frac{\delta}{2}$, such that $\phi(t) > \frac{1}{2}\phi(t_0) = \frac{1}{2e}$ for all $t \in (t_0 - \epsilon, t_0 + \epsilon)$, so

$$\int_a^b f(t)\phi(t)\,dt = \int_{t_0-\frac{\delta}{2}}^{t_0+\frac{\delta}{2}} f(t)\phi(t)\,dt \geq \int_{t_0-\epsilon}^{t_0+\epsilon} f(t)\phi(t)\,dt \geq \frac{c\epsilon}{2e} > 0.$$

But this is in contradiction with $\int_a^b f(t)\phi(t)\,dt = 0$, so it must follow that $f \equiv 0$. □

Corollary 2.14. *A curve $\gamma \in C^1([a,b];\mathbb{R}^n)$ is an extremal if and only if*

$$\frac{\partial \mathcal{L}}{\partial x^i}(t,\gamma(t),\dot\gamma(t),) - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial v^i}(t,\gamma(t),\dot\gamma(t)) = 0 \quad \text{for all } 1 \leq i \leq n \text{ and } t \in [a,b]. \tag{2.6}$$

Proof. Follows by combining Theorem 2.12 with Lemma 2.13, where we consider paths h with $h^i(t) = \phi(t)$, $\phi \in C_0^\infty([a,b];\mathbb{R})$, and $h^j(t) = 0$ for $j \neq i$. □

The equations (2.6) are called the *Euler–Lagrange equations* corresponding to $\mathcal{L}$.

Example 2.6. *The length of paths $\gamma \in C^1([a,b];\mathbb{R}^n)$ is given by the functional:*

$$\mathcal{S}(\gamma) = \int_a^b \sqrt{|\dot\gamma|^2(t)}\,dt.$$

Hence $\mathcal{S}$ is an action with Lagrangian $\mathcal{L}(t,\mathbf{x},\mathbf{v}) = \sqrt{|\mathbf{v}|^2}$. The solution to the Euler–Lagrange equations must correspond to extrema of the length. In Problem Sheet 4, you will show that solutions to the Euler–Lagrange equation are straight lines or constant paths and they are in fact minima of the action.

When we considered Newton's equation, we saw that the equation does not in general remain valid with the same force functions $\mathbf{F}_i$ when performing a coordinate transformation. The change in the force function can be very complicated. Indeed, if this invariance property is satisfied with respect to Galilean coordinate transformations, we said that the force satisfies the principle of Galilean relativity.

The proposition below illustrates that in the case of the Euler–Lagrange equations, the change in the Lagrangian function is not so complicated. First, we will redefine slightly the domain of our Lagrangian, to allow for time-dependent coordinate transformations. Let $\mathcal{L} : \mathbb{R}^{n+1} \times \mathbb{R}^{n+1} \to \mathbb{R}$, then the action takes the form: for $\gamma \in C^1([a,b];\mathbb{R}^n)$

$$\mathcal{S}(\gamma) = \int_a^b \mathcal{L}((t,\gamma(t)),(1,\dot\gamma(t)))\,dt.$$

Proposition 2.15. *Let U, V be open subsets of $\mathbb{R}^n$ and $I, J \subset$ open intervals in $\mathbb{R}$. Let $\{x^\mu\}_{\mu\in\{0,\dots,n\}}$ denote a coordinate chart on $I \times U$. Let $\Psi : I \times U \to J \times V$ be a smooth diffeomorphism, such that $\Psi^0(x) = x^0 =: t$ and denote $y^i = \Psi^i(x)$. Then (2.6) hold with respect to $\{x^\mu\}$ and $\mathcal{L} : I\times U\times\mathbb{R}^{n+1} \to \mathbb{R}$ along $\gamma \in C^1([a, b]; U)$ if and only if for all $1 \le i \le n$*

$$\frac{\partial\widetilde{\mathcal{L}}}{\partial y^i}\left(\Psi(t,\gamma(t)),\begin{pmatrix}1\\ \dot{(\Psi\circ\gamma)}(t)\end{pmatrix}\right) - \frac{d}{dt}\frac{\partial\widetilde{\mathcal{L}}}{\partial w^i}\left(\Psi(t,\gamma(t),\begin{pmatrix}1\\ \dot{(\Psi\circ\gamma)}(t)\end{pmatrix}\right) = 0,$$

with $\widetilde{\mathcal{L}} : J \times V \times \mathbb{R}^{n+1} \to \mathbb{R}$, $\widetilde{\mathcal{L}}(y, w) = \mathcal{L}\left(\Psi^{-1}(y), D\Psi^{-1}(y)w\right)$.

Proof. This will follows from a later, more general discussion of Lagrangians on manifolds. □

For the sake of notational convenience, we will often drop the tilde in $\widetilde{\mathcal{L}}$ when changing coordinates. We will later also see that, in the context of spacetime manifolds $\mathbb{R}\times\mathcal{M}$, it is more natural to define Lagrangians as maps $\mathcal{L} : T(\mathbb{R}\times\mathcal{M}) \to \mathbb{R}$ and the coordinate representations of $\mathcal{L}$ are related by the expression in Proposition 2.15.

Example 2.7. *Let $\Phi : \mathbb{R}_t \times (0,\infty)_r \times (0,\pi)_\theta \times (0,2\pi)_\varphi \to \mathbb{R}_t \times \mathbb{R}^3_{\mathbf{x}}$, be defined as follows:*

$$\begin{aligned}\Phi^0(t, r, \theta, \varphi) &= t,\\ \Phi^1(t, r, \theta, \varphi) &= r\cos\varphi\sin\theta\\ \Phi^2(t, r, \theta, \varphi) &= r\sin\varphi\sin\theta,\\ \Phi^3(t, r, \theta, \varphi) &= r\cos\theta.\end{aligned}$$

Then $\Phi : \mathbb{R}_t \times (0,\infty)_r \times (0,\pi)_\theta \times (0,2\pi)_\varphi \to \Phi(\mathbb{R}_t \times (0,\infty)_r \times (0,\pi)_\theta \times (0,2\pi)_\varphi)$ is a diffeomorphism and $\Psi = \Phi^{-1}$ corresponds to the spherical coordinate chart on a subset of $\mathbb{R}^3$.

Consider the Lagrangian $\mathcal{L}(x, v) = \frac{1}{2}m|\mathbf{v}|^2 - U(|\mathbf{x}|)$ with $U \in C^2((0,\infty))$. Then

$$\widetilde{\mathcal{L}}((t, r, \theta, \varphi), w) = \mathcal{L}(\Phi(t, r, \theta, \varphi), (D\Phi)(t, r, \theta, \varphi)w) = \frac{1}{2}m(D\Phi(t, r, \theta, \varphi)w)^i(D\Phi(t, r, \theta, \varphi)w)_i - U(r)$$

where

$$(D\Phi)(t, r, \theta, \varphi)w = \begin{pmatrix} w^0\\ \cos\varphi\sin\theta w^r - r\sin\varphi\sin\theta w^\varphi + r\cos\varphi\cos\theta w^\theta\\ \sin\varphi\sin\theta w^r + r\cos\varphi\sin\theta w^\varphi + r\sin\varphi\cos\theta w^\theta\\ \cos\theta w^r - r\sin\theta w^\theta\end{pmatrix}$$

so, one can easily verify that:

$$(D\Phi(t, r, \theta, \varphi)w)^i(D\Phi(t, r, \theta, \varphi)w)_i = (w^r)^2 + r^2(w^\theta)^2 + r^2\sin^2\theta(w^\varphi)^2,$$

so

$$\widetilde{\mathcal{L}}((t, r, \theta, \varphi), w) = \frac{1}{2}m((w^r)^2 + r^2(w^\theta)^2 + r^2\sin^2\theta(w^\varphi)^2) - U(r).$$

2.4 Lagrangian mechanics

In the theorem below we show that we can arrive at Newton's equations by considering the Euler–Lagrange equations with respect to an appropriate Lagrangian.

Theorem 2.16 (Hamilton's principle of least action[3])**.** *Consider an N-particle system with conservative forces:*

$$m_A\ddot{\mathbf{x}}_A(t) = -\nabla_{\mathbf{x}_A}U(\mathbf{x}_1(t), \dots, \mathbf{x}_N(t)) \quad 1 \le A \le N, \tag{2.7}$$

[3]Since the extremal of the action need not be a minimum, the principle of least action is somewhat of a misnomer. A more fitting name would have been the principle of stationary action.

for some $U \in C^2(\mathbb{R}^{3N})$. Then a path $\mathbb{R} \supseteq I \ni t \mapsto (\mathbf{x}_1, \dots, \mathbf{x}_N)^T(t)$, with $I \subseteq \mathbb{R}$ and open interval, is a solution to (2.7) if and only it is an extremal of an action $\mathcal{S}$ on I with the Lagrangian $\mathcal{L} : \mathbb{R}^{3N} \times \mathbb{R}^{3N} \to \mathbb{R}$ defined as follows:

$$\mathcal{L}(\mathbf{x}_1, \dots, \mathbf{x}_N, \mathbf{v}_1, \dots, \mathbf{v}_N) = \frac{1}{2} \sum_{A=1}^{n} m_A |\mathbf{v}_A|^2 - U(\mathbf{x}_1, \dots, \mathbf{x}_N).$$

We denote with $T(\dot{\mathbf{x}}_1(t), \dots, \dot{\mathbf{x}}_N(t)) = \frac{1}{2} \sum_{A=1}^{N} m_A |\dot{\mathbf{x}}_A|^2(t)$ the kinetic energy *of the system and $U(\mathbf{x}_1(t), \dots, \mathbf{x}_N(t))$ is the* potential energy*.*

Proof. Consider a path $\gamma : t \mapsto (\mathbf{x}_1, \dots, \mathbf{x}_N)^T(t)$ on I. Then γ is an extremal between $\gamma(t_1)$ and $\gamma(t_2)$, with $t_1, t_2 \in I$ arbitrary, if and only if the E–L equations

$$\left[\frac{\partial \mathcal{L}}{\partial x_A^j}(\gamma(t), \dot{\gamma}(t)) - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial v_A^j}(\gamma(t), \dot{\gamma}(t)) \right] = 0$$

hold on I for all $1 \leq j \leq 3$ and $A = 1, \dots, N$. Let

$$\mathcal{L}(\mathbf{x}_1, \dots, \mathbf{x}_N, \mathbf{v}_1, \dots, \mathbf{v}_N) = \frac{1}{2} \sum_{A=1}^{N} m_A |\mathbf{v}_A|^2 - U(\mathbf{x}_1, \dots, \mathbf{x}_N).$$

Then the E–L equations are equivalent to:

$$-\partial_{x_A^j} U(\mathbf{x}_1(t), \dots, \mathbf{x}_N(t)) - \frac{d}{dt}(m_A \dot{x}_A^j(t)) = 0,$$

which is equivalent to (2.7). □

The Lagrangian approach to mechanics has several key advantages over the Newtonian approach:

1. From Proposition 2.15, it follows that the Euler-Lagrange equations are "covariant" (maintain the same form) under very general coordinate changes. This is in contrast with Newton's equations (2.7), which are only covariant under Galilean coordinate transformations if the principle of Galilean relativity holds. This means it is easier to work in coordinates that are naturally adapted to the physical problem under consideration, which need not be inertial, without having to change the form of the equations.

2. Due to its coordinate independence, the Langrangian approach can be considered on manifolds (which do not come with a preferred coordinate chart). This makes it more natural to consider the motion of particles constrained to a submanifold.

3. The Lagrangian approach generalizes to the setting of equations of motions of *fields*, e.g. electromagnetic fields.

We will make use of the following nomenclature: $q_A^i = x_A^i$ are the *generalized coordinates*, $\dot{q}_A^i = \dot{x}_A^i$ are the *generalized velocity coordinates*, $(p_A)_i = \frac{\partial \mathcal{L}}{\partial v_A^i}$ are the *generalized momentum coordinates* and $\frac{\partial \mathcal{L}}{\partial q_A^i}$ are the *generalized force coordinates*, with $A = 1, \dots, N$ labelling the particle. The Euler–Lagrange equations then take the form:

$$\dot{(p_A)}_i = \frac{\partial \mathcal{L}}{\partial q_A^i}.$$

Example 2.8 (Free particle)**.** *For a free particle, $U = 0$ and $T(\mathbf{v}) = \frac{1}{2} m |\mathbf{v}|^2$. The Euler–Lagrange equations then give:*

$$0 = \frac{d}{dt} \left(\frac{1}{2} m \frac{\partial}{\partial v^i} \sum_{j=1}^{3} (v^j)^2 |_{v=\dot{q}(t)} \right) = m \ddot{q}^i(t)$$

and the generalized momenta are $p_i = m \dot{q}_i$.[4] *Note that $\dot{p}_i = 0$, so the generalized momenta are conserved in time and correspond to the components of the linear momentum.*

[4] You may ignore the placement of indices (superscript/subscript) for now.

In the problem sheets, you will see that the solutions to the E–L equations corresponding to $\mathcal{L}(t, \mathbf{x}, \mathbf{v}) = \frac{1}{2}m|\mathbf{v}|^2$ *must correspond to minimizers of the length between any two fixed points (and are therefore straight lines).*

Example 2.9 (Particle with a central force)**.** *Consider the map from polar to Cartesian coordinates on* $\mathbb{R}^2$*:* $\Phi : (0,\infty)_r \times (0, 2\pi)_\varphi \to \mathbb{R}^2$*, with* $\Phi^1(r,\varphi) = r\cos\varphi$ *and* $\Phi^2(r,\varphi) = r\sin\varphi$*. Consider the Lagrangian* $\mathcal{L}(\mathbf{x}, \mathbf{v}) = \frac{1}{2}m|\mathbf{v}|^2 - U(|\mathbf{x}|)$*. Then we can express with respect to polar coordinates* $q^1 = r$*,* $q^2 = \varphi$ *with* $w = (w^r, w^\varphi)$

$$\mathcal{L}((r,\varphi), w) = \mathcal{L}(\Phi(r,\varphi), D\Phi(r,\varphi)w) = \frac{1}{2}m((w^r)^2 + r^2(w^\varphi)^2) - U(r).$$

The generalized momenta of a particle are then $p_r = m\dot{r}$ *and* $p_\varphi = mr^2\dot{\varphi}$ *and they satisfy the equations:*

$$\begin{aligned}\dot{p}_r &= mr\dot{\varphi}^2 - U'(r),\\ \dot{p}_\varphi &= 0.\end{aligned}$$

By the second equation, we immediately obtain conservation of p_φ *in time, so we can write* $mr^2\dot{\varphi} = L$*, for some* $L \in \mathbb{R}$*. This corresponds precisely to the conservation of angular momentum in time; see (2.4)). Plugging this into the first equation gives:*

$$m\ddot{r} = \frac{L^2}{mr^3} - U'(r).$$

Motivated by (2.9), we say a generalized coordinate q^i is *cyclic* if $\mathcal{L}$ is independent of q^i. It follows immediately by the Euler–Lagrange equations that the corresponding generalized momentum p_i is conserved in time. This may be thought of as a generalization of the conservation of linear and angular momentum in Example 2.8 and 2.9, respectively.

2.5 Hamiltonian mechanics

We will now consider yet another reformulation of Newtonian mechanics called *Hamiltonian mechanics*. This approach can be motivated by its connection with quantum mechanics that we will see later in the course. It is also more convenient for making statements about complicated mechanical systems, like those arising in celestial mechanics, and it connects to the more general theory of dynamical systems, as well as ergodic theory, which is the study of statistical properties of dynamical systems.

Definition 2.7. *A function* $f : \mathbb{R} \supseteq I \to \mathbb{R}$*, with* I *an interval, is* convex *if for all* $x, y \in I$ *and* $t \in [0,1]$

$$f(tx + (1-t)y) \le tf(x) + (1-t)f(y).$$

The function is strictly convex *if the inequality is strict. Similarly, we say a function is (strictly) concave if the inequality is reversed.*

We can extend the notions of convexity/concavity to $f : \mathbb{R}^n \supseteq X \to \mathbb{R}$*, with* X *a convex subset, i.e. if* $x, y \in X$ *then the line segment connecting* x, y *lies in* X*.*

One can show that all convex functions on open convex subsets of $\mathbb{R}^n$ are locally Lipschitz continuous.

Exercise: Convince yourself of this when $n = 1$ by considering $x < w < z < y$ and comparing $\frac{f(z)-f(w)}{z-w}$ with $\frac{f(y)-f(x)}{y-x}$.

Definition 2.8. *Let* $X \subseteq \mathbb{R}^n$ *and* $f : X \to \mathbb{R}$ *be convex. Then the* Legendre transform *of* f *is defined as the function* $f^* : \mathbb{R}^n \supseteq P \to \mathbb{R}$*, with*

$$f^*(p) = \sup_{x\in X}(\langle x, p\rangle - f(x)),$$

with $P = \{y \in \mathbb{R}^n \mid \sup_{x\in X}(\langle x, y\rangle - f(x)) < \infty\}$.

In the proposition below we state some useful properties of the Legendre transform.

Proposition 2.17. *Let* $X \subseteq \mathbb{R}^n$ *and* $f : X \to \mathbb{R}$ *be convex. Let* $f^* : \mathbb{R}^n \supseteq P \to \mathbb{R}$ *be the Legendre transform of* f*. Then:*

(i) *Let f be twice differentiable and strictly convex and assume that for all $p \in P$ there exists an $x_* \in X$ such that $\sup_{x\in X}\langle x, p\rangle - f(x) = \langle x_*, p\rangle - f(x_*)$. Then x_* is unique,*

$$f^*(p) = \langle p, x_*\rangle - f(x_*),$$

with $p = Df(x_*)$ and $P = Df(X)$. Assume that the inverse $(Df)^{-1} : \mathbb{R}^n \supseteq Df(X) \to X$ is well-defined. Then $x_*(p) = (Df)^{-1}(p)$. Furthermore, f^* is twice differentiable with

$$Df^*(p) = x_*(p).$$

(ii) *Assume $P \neq \emptyset$. Then P and f^* are convex.*

(iii) *Let f satisfy the assumptions in* (i). *Then the Legendre transform is involutive, i.e. $(f^*)^* = f$.*

Proof. (Non-examinable)"(i)": By differentiability and convexity of f, x_* corresponds to critical points of $\langle p, x\rangle - f(x)$ and hence $p_i = \partial_i f(x_*)$.

Suppose there exist $x_1, x_2 \in X$ such that $Df(x_1) = Df(x_2)$ and $x_1 \neq x_2$. Since $x_2 - x_2 \neq 0$, we can consider the directional derivatives:

$$\begin{aligned} Df(x_1)(x_2 - x_1) &= \frac{d}{dt}\Big|_{t=0} f(x_1 + t(x_2 - x_1)) = \frac{d}{dt}\Big|_{t=0} f(tx_2 + (1-t)x_1), \\ Df(x_2)(x_2 - x_1) &= -\frac{d}{dt}\Big|_{t=0} f(x_2 - t(x_2 - x_1)) = -\frac{d}{dt}\Big|_{t=0} f(tx_1 + (1-t)x_2). \end{aligned}$$

By subtracting the above equations and using that $Df(x_1) = Df(x_2)$, we therefore get:

$$\begin{aligned} 0 &= \frac{d}{dt}\Big|_{t=0} [f(tx_2 + (1-t)x_1) + f(tx_1 + (1-t)x_2)] \\ &\overset{\text{strict convexity}}{<} \frac{d}{dt}\Big|_{t=0} [tf(x_2) + (1-t)f(x_1) + tf(x_1) + (1-t)f(x_2)] = \frac{d}{dt}\Big|_{t=0} (f(x_2) + f(x_1)) \\ &= 0, \end{aligned}$$

which is a contradiction. Hence, given $p \in P$, there is a unique x_* such that $p = Df(x_*)$.

We will now prove $P = Df(X)$. By the above, $P \subseteq Df(X)$, so it remains to show that for all $x \in X$, $Df(x) \in P$, i.e. for all $y \in X$:

$$\langle Df(x), x\rangle - f(x) \geq \langle Df(x), y\rangle - f(y),$$

which is equivalent to showing that

$$f(x) - f(y) \leq \langle Df(x), (x - y)\rangle. \tag{2.8}$$

Define $g(t) = f(tx + (1-t)y)$. Then, by the mean value theorem, there exists $t_* \in [0, 1]$ such that

$$g(1) - g(0) = g'(t_*).$$

We can obtain (2.8), if we can show that $g'(1) \geq g'(t_*)$. We will use that g must be convex (Exercise) and hence,

$$\frac{g(t_4) - g(t_3)}{t_4 - t_3} \geq \frac{g(t_2) - g(t_1)}{t_2 - t_1}$$

for $t_1 < t_2 < t_3 < t_4$. (Exercise). Either $t_* = 1$, in which case there is nothing to prove, or $t_* < 1$, so

$$g'(1) = \lim_{h\downarrow 0} \frac{g(1+h) - g(1)}{h} \geq \lim_{h\downarrow 0} \frac{g(t_* + h) - g(t_*)}{h} = g'(t_*).$$

The derivative of f^* is given by:

$$\partial_{p_i} f^*(p) = \partial_{p_i}(p_j x_*^j(p) - f(x_*(p))) = x_*^i(p) + p_j \partial_{p_i}(x_*)^j(p) - \overbrace{\partial_{x^j} f(x_*(p))}^{=p_j} \partial_{p_i}(x_*)^j(p) = x_*^i(p),$$

where we used that x_* is differentiable as a function on P, since $x_*(p) = (Df)^{-1}(p)$ and f is twice differentiable. Note however that in passing from f to f^* we do not lose derivatives as the derivatives of x_* in p cancel out.

Property (ii) is the statement that P (non-empty) and f^* are convex. Let $p_1, p_2 \in P$. Then

$$\begin{aligned} f^*(tp_1 + (1-t)p_2) &= \sup_{x\in X} \langle tp_1 + (1-t)p_2, x\rangle - f(x) \\ &= \sup_{x\in X} t(\langle p_1, x\rangle - f(x)) + (1-t)(\langle p_2, x\rangle - f(x)) \\ &\leq t \sup_{x\in X}(\langle p_1, x\rangle - f(x)) + (1-t)\sup_{x\in X}(\langle p_2, x\rangle - f(x)) \\ &= tf^*(p) + (1-t)f^*(p_2) < \infty. \end{aligned}$$

This implies that $tp_1 + (1-t)p_2 \in P$, which means P is convex, and also shows that $f^*(tp_1 + (1-t)p_2) \leq tf^*(p) + (1-t)f^*(p_2)$, which means that f^* is convex.

Property (iii) is the statement that $(f^*)^* = f$, under the conditions of property (i). By property (i), we have the domain of $(f^*)^*$ is $Df^*(P)$ and $q \in Df^*(P)$ implies that $q \in Df^*(P) = (Df)^{-1}(Df(X)) = X$. We also have that

$$(f^*)^*(q) = \langle q, (Df^*)^{-1}(q)\rangle - f^*((Df^*)^{-1}(q)).$$

Note moreover that $(Df^*)^{-1}(q) = Df(q)$, so

$$(f^*)^*(q) = \langle q, Df(q)\rangle - f^*(Df(q)) = \langle q, Df(q)\rangle - (\langle q, Df(q)\rangle - f(q)) = f(q).$$

□

Consider a Lagrangian $\mathcal{L} : \mathbb{R}_t \times \mathbb{R}^n_{\mathbf{x}} \times \mathbb{R}^n_{\mathbf{v}} \to \mathbb{R}$ that is convex with respect to the velocity variable. Then the *Hamiltonian* $H : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is defined as the Legendre transform $\mathcal{L}^*$ with respect to the velocity variable in $\mathbb{R}^n$:

$$H(t, q^1, \ldots, q^n, p_1, \ldots, p_n) = \sup_{v\in\mathbb{R}^n} \langle v, p\rangle - \mathcal{L}(t, q^1, \ldots, q^n, v^1, \ldots, v^n).$$

Suppose $\mathcal{L}$ is differentiable and the above supremum is attained at some value $v_*(t, q, p) \in \mathbb{R}^n$. Then, the identity $p_i = \frac{\partial \mathcal{L}}{\partial v^i}(t, q^1, \ldots, q^n, v^1_*, \ldots, v^n_*)$ holds and:

$$H(t, q, p) = \langle v_*(t, q, p), p\rangle - \mathcal{L}(t, q, v_*(t, q, p)).$$

Theorem 2.18. *Let $\mathcal{L} : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ be a C^2 Lagrangian so that $\mathcal{L}(t, q, \cdot)$ satisfies the assumptions in* (i) *of Proposition 2.17 for all $t \in \mathbb{R}$ and $q \in \mathbb{R}^n$. Then the n-dimensional system of Euler–Lagrange equations along a path $t \mapsto q(t)$*

$$\frac{\partial \mathcal{L}}{\partial q^i}(t, q(t), \dot{q}(t)) - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial v^i}(t, q(t), \dot{q}(t)) = 0$$

are equivalent to the following $2n$-dimensional system of equations involving the twice differentiable Hamiltonian H:

$$\dot{p}_i(t) = -\frac{\partial H}{\partial q^i}(t, q(t), p(t)), \tag{2.9}$$

$$\dot{q}^i(t) = \frac{\partial H}{\partial p_i}(t, q(t), p(t)), \tag{2.10}$$

provided $p_i(t) = \frac{\partial \mathcal{L}}{\partial v^i}(t, q(t), \dot{q}(t))$, i.e. $t \mapsto p_i(t)$ correspond to generalized momenta associated to $\mathcal{L}$.

Equations (2.9) *and* (2.10) *are called the* Hamilton equations.

Proof. Let $t \mapsto q(t)$ be a path. Let $p_i(t) = \frac{\partial \mathcal{L}}{\partial v^i}(t, q(t), \dot{q}(t))$. By the identities $p = Df(x_*)$ and $x_* = (Df^*)(p)$ in (i) of Proposition 2.17, we have that $v^i_*(t, q, p) = \frac{\partial H}{\partial p^i}(t, q, p)$, we can therefore alternatively express the corresponding path $t \mapsto p(t)$ as follows

$$p_i(t) = \frac{\partial \mathcal{L}}{\partial v^i}(t, q(t), v_*(t, q(t), p(t))) = \frac{\partial \mathcal{L}}{\partial v^i}(t, q(t), \nabla_p H(t, q(t), p(t)))$$

Then we must have that

$$\frac{\partial \mathcal{L}}{\partial v^i}(t, q(t), \dot{q}(t)) = \frac{\partial \mathcal{L}}{\partial v^i}(t, q(t), \nabla_p H(t, q(t), p(t))).$$

Since the derivative of $\mathcal{L}(t, q, \cdot)$ is invertible for all t and q, by the assumptions in (i) of Proposition 2.17, it is injective and the above identity implies that

$$\dot{q}^i(t) = v_*^i(t, q(t), p(t)) = \frac{\partial H}{\partial p^i}(t, q(t), p(t)).$$

Hence, the Hamilton equations for q^i must hold.

Since $H(t, q, p) = \langle v_*(t, q, p), p\rangle - \mathcal{L}(t, q, v_*(t, q, p))$, we also have by the chain rule that

$$\begin{aligned}\frac{\partial H}{\partial q^i}(t, q, p) &= \frac{\partial v_*^j}{\partial q^i}(t, q, p)p_j - \frac{\partial \mathcal{L}}{\partial q^i}(t, q, v_*(t, q, p)) - \frac{\partial \mathcal{L}}{\partial v^j}(t, q, v_*(t, q, p))\frac{\partial v_*^j}{\partial q^i}(t, q, p)\\ &= -\frac{\partial \mathcal{L}}{\partial q^i}(t, q, \nabla_p H(t, q, p)) + \frac{\partial^2 H}{\partial q^i \partial p^j}(t, q, p)\left[p_j - \frac{\partial \mathcal{L}}{\partial v^i}(t, q, \nabla_p H(t, q, p))\right]\\ &= -\frac{\partial \mathcal{L}}{\partial q^i}(t, q, \nabla_p H(t, q, p)),\end{aligned}$$

where we used that the term in square brackets vanishes as a result of the relation between p and $\nabla_v \mathcal{L}(t, q, v)$.

Now we evaluate the right-hand side along the path $t \mapsto (q(t), p(t))$:

$$\frac{\partial H}{\partial q^i}(t, q(t), p(t)) = -\frac{\partial \mathcal{L}}{\partial q^i}(t, q(t), \dot{q}(t)).$$

If we now suppose that $t \mapsto q(t)$ satisfies the Euler–Lagrange equations, then

$$\frac{\partial H}{\partial q^i}(t, q(t), p(t)) = -\frac{\partial \mathcal{L}}{\partial q^i}(t, q, \dot{q}(t)) = -\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial v^i}(t, q(t), \dot{q}(t)) = -\dot{p}_i(t),$$

and we conclude that the Hamilton equations hold.

Conversely, suppose that the Hamilton equations hold, then we obtain

$$\dot{p}_i(t) = -\frac{\partial H}{\partial q^i}(t, q(t), p(t)) = \frac{\partial \mathcal{L}}{\partial q^i}(t, q, \dot{q}(t)),$$

which is equivalent to the Euler–Lagrange equations, if we use that $p_i(t) = \frac{\partial \mathcal{L}}{\partial v^i}(t, q(t), \dot{q}(t))$. □

Along a solution $t \to q(t)$ to the E–L equations corresponding to a system of particles with a conservative force, $H(t, q(t), p(t))$ with $p_i(t) = \frac{\partial \mathcal{L}}{\partial \dot{q}^i}(t, q(t), \dot{q}(t))$ gives the value of the total energy of the system at time t:

Proposition 2.19. *Let $\mathcal{L}(t, q, v) = T(v) - U(q) = \frac{1}{2}m|v|^2 - U(q)$ with $m > 0$ and $U \in C^2(\mathbb{R}^n)$. Then $H(q, p) = T(v_*(q, p)) + U(q)$. In particular, if $t \mapsto (q(t), p(t))$ is a solution to (2.9)–(2.10), then $H(q(t), p(t)) = E_q(t)$, i.e. the Hamiltonian evaluated along the motion agrees with its energy.*

Proof. One can easily verify that $\mathcal{L}(t, q, v)$ is C^2 and strictly convex in v and that the supremum in the definition of its Legendre transform in v is attained. Hence the Hamiltonian H is well-defined and

$$\begin{aligned}H(t, q, p) = p_i(v_*(q, p))^i - (T(v_*(q, p)) - U(q)) &= \frac{\partial \mathcal{L}}{\partial v^i}(t, q, v_*(q, p))(v_*(t, q, p))^i - \frac{m}{2}|v_*(q, p)|^2 + U(q)\\ &= T(v_*(q, p)) + U(q).\end{aligned}$$

If $t \mapsto (q(t), p(t))$ satisfy (2.9)–(2.10), then $v_*(q(t), p(t)) = \dot{q}(t)$ from which $H(q(t), p(t)) = T(\dot{q}(t)) + U(q(t)) = E_q(t)$ follows. □

Conservation of energy (Proposition 2.9) takes the following form in the (more general) Hamiltonian setting:

Proposition 2.20. *Let H be a Hamiltonian with $\partial_t H(t,q,p) = 0$. If $t \mapsto (q(t),p(t))$ is a solution to the Hamilton equations (2.9)–(2.10), then the map $t \mapsto H(t,q(t),p(t))$ is constant.*

Proof.

$$\frac{d(H\circ(q,p))}{dt}(t) = \frac{\partial H}{\partial q^i}(t,q(t),p(t))\dot{q}^i(t) + \frac{\partial H}{\partial p_i}(t,q(t),p(t))\dot{p}_i(t) + \partial_t H(t,q(t),p(t)) = -\dot{p}_i(t)\dot{q}^i(t) + \dot{p}_i(t)\dot{q}^i(t) = 0.$$

□

In the proposition below, we show that we can reduce the dimension of the system of Hamilton equations (the degrees of freedom) from $2n$ to $2(N-1)$, if we can identify a cyclic coordinate. This is a characteristic feature of the Hamiltonian formalism.

Proposition 2.21. *Let $H : \mathbb{R}\times\mathbb{R}^n\times\mathbb{R}^n \to \mathbb{R}$ be a Hamiltonian with a cyclic coordinate q^1. Then a solution to the Hamilton equations $t \mapsto (q(t),p(t))$ satisfies $p_1(t) = p(0)$ for all t and $t \mapsto (q^2,\dots,q^n,p_2,\dots p_n)$ satisfies the Hamilton equations with respect to the reduced Hamiltonian H_{p_1}, which is parametrized by the constant p_1 and is defined as follows:*

$$H_{p_1}(t,q_2,\dots,q_n,p_2,\dots p_n) := H(t,0,q_2,\dots,q_n,p_1(0),p_2,\dots p_n),$$

Proof. It follows immediately from (2.9)–(2.10) that:

$$\begin{aligned}\dot{p_1} &= -\frac{\partial H}{\partial q^1} = 0,\\ \dot{q_1} &= \frac{\partial H}{\partial p_1},\end{aligned}$$

so $t \mapsto p_1(t)$ is constant and p_1 can be treated as a parameter. The Hamilton equations for H_{p_1}

$$\begin{aligned}\frac{\partial H_{p_1}}{\partial q^i} &= \frac{\partial H}{\partial q^i} = -\dot{p}_i \quad 2\le i\le n,\\ \frac{\partial H_{p_1}}{\partial p_i} &= \frac{\partial H}{\partial p_i} = \dot{q}_i \quad 2\le i\le n.\end{aligned}$$

After solving the above equations, we simply integrate the equation for $\dot{q}_1$ to obtain:

$$q_1(t) = q_1(0) + \int_0^t \frac{\partial H_{p_1}}{\partial p_1}(t,q_2(t),\dots,q_n(t),p_2(t),\dots,p_n(t))\,dt.$$

□

We refer to the $2n$-dimensional space of coordinates and momenta $(q^1,\dots,q^n,p_1,\dots p_n)$ as *phase space*. In the context of Hamiltonian mechanics on manifolds arising from Lagrangian mechanics, it is given by the cotangent bundle:

$$T^*\mathcal{M}.$$

It is however possible to study Hamiltonian equations on more general even-dimensional manifolds.

2.6 Symplectic manifolds

A more geometric approach to studying Hamiltonian systems can be obtained by considering *symplectic manifolds*, which are even-dimensional manifolds $\mathcal{M}$ equipped with a symplectic form, which is a closed, non-degenerate 2-form $\omega \in \Omega^2(\mathcal{M})$.

This means: 1) at each $x \in \mathcal{M}$, $\omega(x)$ is an anti-symmetric bilinear form, 2) let $X_x, Y_x \in T_x\mathcal{M}$, if $\omega(x)(X_x,Y_x) = 0$ for all $Y_x \in T_x\mathcal{M}$, then $X_x = 0$ (non-degeneracy, and 3) $d\omega = 0$ (closedness).

The non-degeneracy and bilinearity of ω implies that for all vector fields $X \in \Gamma(T\mathcal{M})$, there exists a unique one form, denotes $X^\flat \in \Omega^1(\mathcal{M})$, such that $X^\flat(Y) = \omega(Y,X)$. The map $\flat : \Gamma(T\mathcal{M}) \to \Omega(\mathcal{M})$ is actually bijective, with inverse $\sharp : \Omega^1(\mathcal{M}) \to \Gamma(T\mathcal{M})$. In the setting of Riemannian and Lorentzian metrics later in the course, we will refer to analogous maps $\flat$ and $\sharp$ as *musical isomorphisms*.

Example 2.10. *The space $(\mathbb{R}^{2n}, \omega)$ with coordinates q^i and p^i, $i = 1, \ldots, n$, and $\omega = \sum_{i=1}^n dp^i \wedge dq^i$ is a symplectic manifold. Given a vector field $X = \sum_{i=1}^n X^i \partial_{q^i} + \tilde{X}^i \partial_{p^i}$, we have that*

$$\omega(Y, X) = \sum_{i=1}^n dq_i(X) dp^i(Y) - dq_i(Y) dp^i(X) = \sum_{i=1}^n X^i dp^i(Y) - \tilde{X}^i dq^i(Y).$$

Hence $X^\flat = \sum_{i=1}^n X^i dp^i - \tilde{X}^i dq^i$.

On any even-dimensional manifold, there exists coordinates so that locally ω takes the same form as in the example above. We will state the relevant theorem without proof.

Theorem 2.22. *(Darboux's theorem) Let $(\mathcal{M}, \omega)$ be a $2n$-dimensional symplectic manifold. At each point $x \in \mathcal{M}$, there exists a neighbourhood U_x which can be covered by a coordinate chart $(q^1, \ldots, q^n, p^1, \ldots, p^n)$ with respect to which ω takes the following form:*

$$\omega = \sum_{i=1}^n dp^i \wedge dq^i.$$

These coordinates are called: Darboux coordinates*,* symplectic coordinates *or* canonical coordinates*.*

Consider a function $H \in C^\infty(\mathcal{M})$, which we will call the Hamiltonian. A particularly important vector field on a symplectic manifold is the *Hamiltonian vector field* $X_H := (dH)^\sharp$. We can locally express with respect to Darboux coordinates (q^i, p^i): $dH = \sum_{i=1}^n \partial_{q^i} H dq^i + \partial_{p^i} H dp^i$. So by Darboux's Theorem, we can express in these coordinates:

$$X_H = \sum_{i=1}^n (\partial_{p^i} H) \partial_{q^i} - (\partial_{q^i} H) \partial_{p^i}.$$

We refer to the triple $(\mathcal{M}, \omega, H)$ as a *Hamiltonian system.*

Recall that orbits of a vector field $X \in \Gamma(T\mathcal{M})$ are curves $\gamma : I \to \mathcal{M}$ such that $T_{\gamma(t)}\mathcal{M} \ni \dot{\gamma}(t) = X(\gamma(t))$. Now, we can give a completely geometric characterization of solutions to Hamilton's equations as orbits $t \mapsto \gamma(t)$ of the Hamiltonian vector field. Indeed, with respect to Darboux coordinates, we have that for $\gamma(t) = (q^i(t), p^i(t))$

$$\begin{aligned} \dot{q}^i(t) &= (\partial_{p^i} H)(\gamma(t)), \\ \dot{p}^i(t) &= -(\partial_{q^i} H)(\gamma(t)). \end{aligned}$$

More generally, we define with $\Phi_t^H : \mathcal{M} \to \mathcal{M}$ the flow for time t with respect to the Hamiltonian vector field X_H, which sends $x \in M$ to $\gamma(t)$, where γ satisfies $\gamma(0) = x$ and $\dot{\gamma}(t) = (X_H)_{\gamma(t)} \in T_{\gamma(t)}\mathcal{M}$.

To connect with quantum mechanics, we will use our geometric reformulation of Hamiltonian systems to define the notion of a *Poisson bracket.*

Definition 2.9. *A Poisson bracket is a binary operation $\{\cdot, \cdot\} : C^\infty(\mathcal{M}) \times C^\infty(\mathcal{M}) \to C^\infty(\mathcal{M})$ defined as follows:*

$$\{f, g\} = \omega(X_f, X_g) = \omega((df)^\sharp, (dg)^\sharp) = df(X_g) = X_g(f).$$

The Poisson bracket with $\{f, g\}$ can be interpreted as measuring the rate of change of f with respect to the Hamiltonian flow corresponding to g. In particular, along $\gamma : I \to \mathcal{M}$ an orbit of X_H, we have that

$$\frac{d}{dt} f(\gamma(t)) = \{f, H\}(\gamma(t)).$$

With respect to Darboux coordinates, we have that

$$\{f, g\} = \sum_{i=1}^n \partial_{q^i} f \partial_{p^i} g - \partial_{p^i} f \partial_{q^i} g.$$

In particular,

$$\{q^i, p^j\} = \delta^{ij}.$$

Let $\rho : \mathbb{R}_t \times \mathcal{M} \to [0, \infty)$ be a density function on $\mathcal{M}$ for all $t \in \mathbb{R}$. Suppose that ρ stays constant along the Hamiltonian flow. Then

$$0 = \frac{d}{dt}\rho(t, \gamma(t)) = (\partial_t \rho)(t, \gamma(t)) + \{\rho(t, \cdot), H\}(\gamma(t)).$$

Rearranging the above terms gives the *Liouville equation*:

$$(\partial_t \rho)(t, \cdot) = -\{\rho(t, \cdot), H\}.$$

The Liouville equation plays an important role in classical statistical mechanics.

We state without proof the key properties of Poisson brackets:

Proposition 2.23. *Let $(\mathcal{M}, \omega)$ be a symplectic manifold and let $f, g, h \in C^\infty(\mathcal{M})$. Then:*

(i) *(bilinearity) $\{f, g\}$ is linear in f and g over $\mathbb{R}$,*

(ii) *(antisymmetry) $\{f, g\} = -\{g, f\}$,*

(iii) *(Jacobi identity) $\{\{f, g\}, h\} + \{\{g, h\}, f\} + \{\{h, f\}, g\} = 0$,*

(iv) $X_{\{f,g\}} = -[X_f, X_g]$.

In particular, the vector space $C^\infty(\mathcal{M})$ is a Lie algebra with respect to the Poisson bracket.

As we will see later in the course, position q^i and momentum q^i will become linear operators and the role of the Poisson bracket will be taken on by the commutator of linear operators, which also satisfies properties (i)–(iii) above.

The symplectic formulation has the advantage that *Liouville's theorem* reduces to a sequence of algebraic identities.

Theorem 2.24 (Liouville's Theorem)**.** *Let $(\mathcal{M}, \omega, H)$ be a Hamiltonian system. Then ω^n defines a volume form on $\mathcal{M}$,*[5] *which is preserved under the Hamiltonian flow, i.e.*

$$L_{X_H}(\omega^n) = 0,$$

with L_{X_H} the Lie derivative with respect to X_H and $\omega^n = \overbrace{\omega \wedge \ldots \wedge \omega}^{n}$. With respect to Darboux coordinates, we have that

$$\frac{1}{n!}\omega^n = dp^1 \wedge dq^1 \wedge dp^2 \wedge dq^2 \wedge \ldots \wedge dp^n \wedge dq^n.$$

Proof. We will apply *Cartan's magic formula*: for any $X \in \Gamma(T\mathcal{M})$

$$L_{X_H} = d \circ \iota_{X_H} + \iota_{X_H} \circ d,$$

where d is the exterior derivative and ι_X, with $X \in \Gamma(T\mathcal{M})$ denotes an interior product: recall, for $r \geq 1$ and $Y \in \Gamma(T\mathcal{M})$,

$$\iota_Y : \Omega^r(\mathcal{M}) \to \Omega^{r-1}(\mathcal{M}),$$
$$(\iota_Y \beta)(X_1, \ldots, X_{r-1}) = \omega(Y, X_1, \ldots, X_{r-1}).$$

Note that $d\omega^k = 0$ for all $k \geq 0$, so

$$L_{X_H}\omega^n = d\iota_{X_H}\omega^n.$$

We have that $\iota_{X_H}\omega^n = \omega(X_H, \cdot)\omega^{n-1} = -dH \wedge \omega^{n-1}$. Taking the exterior derivative d then gives zero.

It follows by an easy induction argument we can locally express in Darboux coordinates, $\frac{1}{n!}\omega^n = dp^1 \wedge dq^1 \wedge \ldots \wedge dp^n \wedge dq^n$. □

[5] Exercise: Convince yourself of this, once you have become familiar with the notion of volume form on general manifolds.

Consider the Hamiltonian system $(\mathbb{R}^{2n}, \sum_{i=1}^n dp^i \wedge dq^i, H)$ where Darboux coordinates are global and let $\Omega \subset \mathbb{R}^{2n}$ be bounded. Let $\Omega_t = \Phi_t^H(\Omega) \subset \mathbb{R}^{2n}$ denote the image of Ω under the Hamiltonian flow. Then Liouville's theorem implies that

$$\frac{d}{dt}\text{Volume}(\Omega_t) = \frac{d}{dt}\int_{\Omega_t} dp^1 dq^1 \dots dp^n dq^n = 0,$$

so the volume of Ω_t is equal to the volume of Ω for all time. Hence, the phase space volume is preserved under the Hamiltonian flow.

Let $\rho : \mathbb{R}_t \times \mathcal{M} \to [0, \infty)$ be a solution to the Liouville equation, such that $\int_{\mathcal{M}} \rho(t, \cdot)\frac{\omega^n}{n!} = 1$ for all $t \in \mathbb{R}$, i.e. we can think of $\rho(t, \cdot)$ as a probability density at time t. It follows by Liouville's theorem, that the probability of encountering a system in the phase space region Ω_t is $\int_{\Omega_t} \rho(t, \cdot)\frac{\omega^n}{n!}$ is invariant under time.

Let $O \in C^1(\mathcal{M})$ represent a measurable quantity (for example, the total kinetic energy). Then we can define the expectation value of O at time t as follows:

$$\langle O \rangle(t) = \int_{\mathcal{M}} O\rho(t, \cdot)\frac{\omega^n}{n!}.$$

By Liouville's equation and Liouville's theorem, and after integrating by parts (assuming ρ decays suitably as infinity or the boundary of $\mathcal{M}$), we have that

$$\frac{d\langle O \rangle}{dt}(t) = \int_{\mathcal{M}} O\partial_t\rho(t, \cdot)\frac{\omega^n}{n!} = -\int_{\mathcal{M}} O\{\rho(t, \cdot), H\}\frac{\omega^n}{n!} = \int_{\mathcal{M}} \{O, H\}\rho(t, \cdot)\frac{\omega^n}{n!} = \langle \{O, H\} \rangle(t).$$

We will encounter similar equations of motions when we study expectation values of observables in quantum mechanics.

As a corollary of Liouville's theorem, can obtain a remarkable result with far-reaching consequences, which really only uses the volume-preserving property of the Hamiltonian flow.

Corollary 2.25 (Poincaré's recurrence theorem)**.** *Let $(\mathcal{M}, \omega, H)$ be a Hamiltonian system and let $\mathcal{K} \subset \mathcal{M}$ be a compact subset, such that $\Phi_t^H(\mathcal{K}) = \mathcal{K}$ for all $t \in \mathbb{R}$.*

Consider an arbitrary $x_0 \in \mathcal{K}$. Then for any neighbourhood U of x_0 and any $T > 0$, there exists a time $t_* > T$ such that the orbit corresponding to the Hamiltonian flow $t \mapsto x(t)$ with $x(0) = x_0$ satisfies $x(t_*) \in U$.

Proof. First of all, note that the volume of $\mathcal{K}$ is bounded with respect to the volume form ω^n. Indeed, consider around each point $x \in \mathcal{M}$ a neighbourhood covered by Darboux coordinates with a bounded range. Then the volume of each neighbourhood is bounded with respect to ω^n. Since $\mathcal{K}$ is compact and is covered by finite-volume Darboux neighbourhoods, it admits a finite subcover, so its volume is finite.

Let $U_t = \Phi_t^H(U)$. Suppose

$$U_t \cap U_s = \emptyset$$

for all $t, s \in \mathbb{R}$ with $t - s > T$. In particular, this means that for any sequence of times $\{t_i\}_{i\in\mathbb{N}}$ such that $t_{i+1} - t_i > T$ for all $i \in \mathbb{N}$, we have that $U_{t_i} \cap U_{t_j} = \emptyset$ for all $i, j \in \mathbb{N}$ with $i \neq j$.

By Liouville's theorem, the volume of each U_{t_i} equals the volume of U. Since the sets are disjoint and contained in $\mathcal{K}$, we therefore have that

$$\infty > \text{Volume}(\mathcal{K}) \geq \text{Volume}\left(\bigcup_{i\in\mathbb{N}} U_{t_i}\right) = \sum_{i\in\mathbb{N}} \text{Volume}(U_{t_i}) = \sum_{i\in\mathbb{N}} \text{Volume}(U) = \infty,$$

which is a contradiction.

There must therefore exist $s, t \in \mathbb{R}$ with $t - s > T$, such that $U_t \cap U_s \neq \emptyset$. Denote $t_* = t - s$, then

$$\Phi_{-s}^H(U_t \cap U_s) = U_{t_*} \cap U \neq \emptyset.$$ □

Poincaré's theorem says that for Hamiltonian systems restricted to a compact subset of phase space and for any initial configuration, the system will get arbitrarily close to its initial configuration after large enough time. A trivial example would be the harmonic oscillator. A counter-intuitive example would be the

following: consider a box with a barrier containing only gas particles on one side of the barrier. Now remove the barrier and the gas particles will start filling the whole box. By Poincaré's recurrence theorem[6], however, all the gas particles will, after some time, move to one side of the barrier again. A resolution of this paradox is that Poincaré's recurrence theorem does not give an upper bound estimate for the time t_*. Therefore, t_* could in principle be much longer than the time scale for which the model is relevant (e.g. greater than the age of the universe).

2.7 Lagrangian mechanics on manifolds

In this section, we will deal with Lagrangian mechanics involving constraints. We will present how to deal with constraints using the language of manifolds and a bit of geometry, and we will show how this relates to Lagrange multipliers.

Consider a C^2 Lagrangian $L : \mathbb{R}_t \times \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}$. Let $n \in \mathbb{N}$, $n < N$ and let

$$\mathcal{M}_t = \{\mathbf{x} \in \mathbb{R}^N \,|\, G(t, \mathbf{x}) = 0\},$$

with $G : \mathbb{R}_t \times \mathbb{R}^N \to \mathbb{R}^{N-n}$ a smooth function. If $DG(t, \mathbf{x})$ is surjective, i.e. it has maximum rank $N - n$ at each $(t, \mathbf{x})$ with $\mathbf{x} \in \mathcal{M}_t$ then $\mathcal{M}_t$ is an n-dimensional embedded submanifold of $\mathbb{R}^N$ for each t by the Rank Theorem (which is a consequence of the Inverse Function Theorem). Equivalently, the vectors $\{\nabla_{\mathbf{x}} G_A(t, \mathbf{x})\}_{1 \leq A \leq N-n}$ are non-zero and linearly independent for each $t \in \mathbb{R}$ and $\mathbf{x} \in \mathcal{M}_t$. The gradients $\{\nabla_{\mathbf{x}} G_A\}_{1 \leq A \leq N-n}$ are normal to $\mathcal{M}_t$. We refer to G as a *constraint function*.

We will refer to the level sets G satisfying the above conditions as a *holonomic constraints*. *Non-holonomic constraints* are systems involving some kind of constraint that can not be described by holonomic constraints (for example G could also depend on a velocity variable).

The above discussion motivates the consideration of Lagrangians on manifolds $\mathcal{M}$:

$$\mathcal{L} : T(\mathbb{R} \times \mathcal{M}) \to \mathbb{R},$$

with $T(\mathbb{R} \times \mathcal{M}) = \coprod_{p \in \mathcal{M}} T_p(\mathbb{R} \times \mathcal{M})$ the tangent bundle of $\mathbb{R} \times \mathcal{M}$ (a disjoint union of tangent spaces).

Defining $\mathcal{L}$ as a map on $T(\mathbb{R} \times \mathcal{M})$ has the further advantage that its manifestly coordinate invariant, so it directly incorporates the desired transformation properties when we change coordinates. We will assume for the sake of simplicity that $\mathcal{L}$ is smooth. Note that the corresponding derivative map $d\mathcal{L}$ is a 1-form on the tangent bundle $T(\mathbb{R} \times \mathcal{M})$, i.e. $d\mathcal{L} \in \Omega^1(T(\mathbb{R} \times \mathcal{M})) = \Gamma(T^*(T(\mathbb{R} \times \mathcal{M})))$.

Given a smooth coordinate chart (U, ψ) with $U \subseteq \mathbb{R} \times \mathcal{M}$, we can express: $\psi = (q^0 = t, q^1, \ldots, q^n) : U \to \mathbb{R}^{n+1}$. Recall that for $q \in U$, we can express any $v_q \in T_q(\mathbb{R} \times \mathcal{M})$ as follows:

$$v_q = v_q^\mu \partial_{q^\mu}|_q,$$

with $\partial_{q^\mu}|_p$ the basis of coordinate vectors at p associated to the chart ψ. Recall also that for $\pi : T(\mathbb{R} \times \mathcal{M}) \to \mathbb{R} \times \mathcal{M}$, with $\pi(q, v_q) = q$ (the projection map), the pair $(\pi^{-1}(U), \phi)$ defines a coordinate chart, with $\phi : \pi^{-1}(U) \to \mathbb{R}^{2(n+1)}$,

$$\phi(q, v_q) = (\psi(q), v_q^0, \ldots, v_q^n).$$

The *coordinate representation of* $\mathcal{L}$ is the map $\widehat{\mathcal{L}} : \mathbb{R}^{2(n+1)} \supseteq \phi(\pi^{-1}(U)) \to \mathbb{R}$ defined by

$$\widehat{\mathcal{L}}(q^0, \ldots, q^n, v^0, \ldots, v^n) = \mathcal{L}(\phi^{-1}(q^0, \ldots, q^n, v^0, \ldots, v^n)).$$

We can also express on $TU = \pi^{-1}(U)$:

$$d\mathcal{L} = \partial_{q^\mu} \mathcal{L} dq^\mu + \partial_{v^\mu} \mathcal{L} dv^\mu,$$

with q^μ and v^μ the components of the chart ϕ on TU.

Suppose $\tilde{\psi}$ is another coordinate chart on U and $\tilde{\phi}$ is the corresponding coordinate chart on $\pi^{-1}(U)$. Let $\widetilde{\mathcal{L}} : \tilde{\phi}(\pi^{-1}(U)) \to \mathbb{R}$ denote the corresponding coordinate representation of $\mathcal{L}$. Then we can express:

$$\widetilde{\mathcal{L}}(\tilde{q}^0, \ldots, \tilde{q}^n, w^0, \ldots, w^n) = \mathcal{L}(\tilde{\phi}^{-1}(\tilde{q}^0, \ldots, \tilde{q}^n, w^0, \ldots, w^n)) = \widehat{\mathcal{L}}((\phi \circ \tilde{\phi}^{-1})(\tilde{q}^0, \ldots, \tilde{q}^n, w^0, \ldots, w^n)) \quad (2.11)$$

[6] When the position space is bounded we also have boundedness in momentum space, assuming boundedness of the potential energy and conservation of energy. We can therefore restrict to a compact subset of phase space.

Denote the corresponding transition function with $\Psi = \tilde{\psi} \circ \psi^{-1} : \mathbb{R}^{n+1} \supseteq \psi(U) \to \tilde{\psi}(U) \subseteq \mathbb{R}^{n+1}$. Then

$$(\phi \circ \tilde{\phi}^{-1})(\tilde{q}^0, \dots, \tilde{q}^n, w^0, \dots, w^n) = \begin{pmatrix} \Psi^{-1}(\tilde{q}^0, \dots, \tilde{q}^n), D\Psi^{-1}(\tilde{q}^0, \dots, \tilde{q}^n) \begin{pmatrix} w^0 \\ \vdots \\ w^n \end{pmatrix} \end{pmatrix}.$$

Theorem 2.26. *Let $\mathcal{M}$ be a smooth n-dimensional manifold and consider the coordinate chart (U, ψ), with $\psi = (t = q^0, q^1, \dots, q^n) : U \to \mathbb{R}^{n+1}$. We consider spacetime paths $\gamma \in C^1([a,b], U)$, such that $\gamma^0(t) = t$. Consider the action $\mathcal{S}(\gamma) = \int_a^b \mathcal{L}(\gamma(t), \dot{\gamma}(t))\, dt$. Then γ is an extremal of $\mathcal{S}$ if and only if*

$$\frac{\partial \mathcal{L}}{\partial q^i}(\gamma(t), \dot{\gamma}(t)) - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial v^i} \circ (\gamma, \dot{\gamma})\right)(t) = 0. \tag{2.12}$$

for all $1 \leq i \leq n$ and $t \in [a,b]$.

Proof. We consider the coordinate representation $\mathcal{L} \circ \phi^{-1}$ on $\phi(U)$, with $\phi : \pi^{-1}(U) \to \mathbb{R}^{2(n+1)}$, $\phi(q, v_q) = (q^0, \dots, q^n, v_q^0, \dots, v_q^n)$, where $v_q = v_q^\mu \partial_{q^\mu}|_q$ and apply the argument from the $\mathcal{M} = \mathbb{R}^n$ setting, using that the consideration of spacetime paths γ with $\gamma^0(t) = t$ is equivalent to considering paths in space (with no time component). □

The above proposition, together with (2.11) implies in particular Proposition 2.15.

We now assume there exists a smooth map $u : \mathbb{R}_t \times \mathcal{M} \to \mathbb{R}_t \times \mathbb{R}^N$, such that $u^0(t, \mathbf{x}) = t$ and $u(t, \cdot)$ defines a smooth embedding of $\mathcal{M}$ into $\{t\} \times \mathbb{R}^N$ for each $t \in \mathbb{R}$. The manifolds $\mathcal{M}_t$ are called *embedded submanifolds*. In the setting of holonomic constraint functions G, the manifolds $\mathcal{M}_t$ are subsets of $\mathbb{R}^n$, so we can simply define u as follows: $u(t, \mathbf{x}) = (t, \mathbf{x})$.

We can relate $\mathcal{L}$ to a different Lagrangian $L : \mathbb{R}_t \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}$, such that for $(q, v) \in T(\mathbb{R}_t \times \mathcal{M})$:

$$\mathcal{L}(q, v) = L(u_*(q, v)).$$

where

$$\begin{aligned} u_* : T(\mathbb{R}_t \times \mathcal{M}) &\to T(\mathbb{R}_t \times \mathbb{R}^N) \cong \mathbb{R}_t \times \mathbb{R}^N \times \mathbb{R}_t \times \mathbb{R}^N, \\ u_*(q, v) &= (u(q), du_q(v)), \\ du_q(v) &= \partial_{q^\mu} u^\alpha(q) v^\mu \partial_{x^\alpha}|_{u(q)} \cong (\partial_{q^\mu} u^0(q) v^\mu, \partial_{q^\mu} u^1(q) v^\mu, \dots, \partial_{q^\mu} u^N(q) v^\mu), \end{aligned}$$

with respect to a coordinate chart $\{q^\mu\}_{0 \leq \mu \leq n}$ on $U \subseteq \mathbb{R}_t \times \mathcal{M}$ and Cartesian coordinates $\{x^\alpha\}_{0 \leq \alpha \leq N}$ on $\mathbb{R}_t \times \mathbb{R}^N$.

If $L(x, v) = \frac{1}{2} m |\mathbf{v}|^2 - U(\mathbf{x})$, then

$$\mathcal{L}(q, v) = \frac{1}{2} m (du_q(v))_i (du_q(v))^i - U(u^1(q), \dots, u^N(q)).$$

Note that $g_t \in \Gamma(T^*\mathcal{M}_t \otimes T^*\mathcal{M}_t)$, with $g_t(\mathbf{q})(v_1, v_2) = (du_{(t,\mathbf{q})}(1, v_1))_i (du_{(t,\mathbf{q})}(1, v_2))^i$ defines a positive-definite symmetric (0,2)-tensor field and $(\mathcal{M}_t, g_t)$ can be viewed as a 1-parameter family of Riemannian manifolds.

Hence, we obtain in this case

$$\mathcal{L}((t, \mathbf{q}), (1, v)^T) = \frac{1}{2} m g_t(\mathbf{q})(v, v) - U(u^1(t, \mathbf{q}), \dots, u^N(t, \mathbf{q})).$$

Now, we return to the study of Lagrangians on $\mathbb{R}_t \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N$ with constraints $G(t, \mathbf{x}) = 0$. By applying the chain rule, the equations (2.12) imply the following equations for L: with respect to a coordinate chart $\{q^\mu\}_{0 \leq \mu \leq n}$ on $U \subseteq \mathbb{R}_t \times \mathcal{M}$ and Cartesian coordinates $\{x^\alpha, w^\alpha\}_{0 \leq \alpha \leq N}$ on $T(\mathbb{R}_t \times \mathbb{R}^N)$, we have that the Euler–Lagrange equations with respect $\mathcal{L}$ for a path $\gamma \in C^1(U)$ give

$$\left[\frac{\partial L}{\partial x^j}(u(\gamma(t)), u\dot{(}\gamma)(t)) - \frac{d}{dt}\left(\frac{\partial L}{\partial w^j}(u(\gamma(t)), u\dot{(}\gamma)(t))\right)\right] \partial_{q^i} u^j(\gamma(t)) = 0 \quad \forall \quad \forall\, 1 \leq i \leq n,$$

where in the above summation $1 \leq j \leq N$.

Note that we used here that $v \mapsto du_q(v)$ is a linear map, so

$$\partial_{v^i}(L(u(q), du_q(v)) = (\partial_{w^\alpha} L)(u(q), du_q(v))\partial_{v^i} du_q^\alpha(v) = (\partial_{w^\alpha} L)(u(q), du_q(v))\partial_{q^i} u^\alpha(q).$$

This implies that the term in square brackets can be interpreted as the components of a vector in $\mathbb{R}^N$ that lies in the kernel of the transpose of the matrix with components $\partial_{q^i} u^j(q)$. Since this kernel is spanned by $\{\nabla G^1(t, \mathbf{x}), \ldots, \nabla G^{N-n}(t, \mathbf{x})\}$, we can express the Euler–Lagrange equations as follows:

$$\left[\frac{\partial L}{\partial x^i}(t, \mathbf{x}(t), \dot{\mathbf{x}}(t)) - \frac{d}{dt}\left(\frac{\partial L}{\partial w^i}(t, \mathbf{x}(t), \dot{\mathbf{x}}(t))\right)\right] = \sum_{j=1}^{N-n} \lambda^j(t)\partial_{x^i} G^j(t, \mathbf{x}) \quad \forall\, 1 \leq i \leq N.$$

The functions λ^j are called *Lagrange multipliers*. Note that these can be interpreted as N equations for N unknowns $q^1(t), \ldots, q^n(t), \lambda^1(t), \ldots, \lambda^{N-n}(t)$. The above equations are equivalent to the standard Euler–Lagrange equations on $\mathbb{R}^N$ for the modified Lagrangian:

$$\mathscr{L}(t, \mathbf{x}, \mathbf{v}, \lambda^1, \ldots, \lambda^{N-n}) = L(t, \mathbf{x}, \mathbf{v}) - \lambda^j G^j(t, \mathbf{x})$$

coupled to the constraint equation $G(t, \mathbf{x}(t)) = 0$ (or equivalently, $\frac{\partial \mathscr{L}}{\partial \lambda^j} = 0$). We then consider the paths $t \mapsto (\mathbf{x}(t), \lambda^1(t), \ldots, \lambda^{N-n}(t))$, which solve the Euler–Lagrange equations and $G(t, \mathbf{x}(t)) = 0$.

We can interpret $\lambda^j(t)G^j(t, \mathbf{x})$ as as kind of potential corresponding to a *constraint force*:

$$\mathbf{F}_{\text{constraint}}(t, \mathbf{x}) = -\lambda^j(t)\nabla_{\mathbf{x}} G^j(t, \mathbf{x})$$

which points in the normal direction to the submanifold determined by G and can be interpreted as keeping the particle constrained to the surface.

We see therefore that the effect of a particles moving in a non-trivial geometry can be interpreted as an additional force in a larger ambient space, and vice versa! Having seen this correspondence between forces and geometry will perhaps remove some of the magic when we pass to the geometric setting of Einstein's theory of gravity and represent idealized, free-falling observers by geodesics in a spacetime manifold.[7]

Example 2.11. *Consider two particles with masses m_1 and m_2, attached to each other via an inextendible, massless string of length l over a massless pulley and initially at rest with negative z-coordinates. You may assume the radius of the pulley is R. We assume a constant gravitational force $F = -m_i g\hat{\mathbf{z}}$. Such a set-up is called an Atwood machine; see Figure 1. We would like to determine the motion of each particle. As the forces acting on the particles point all point in the $\hat{\mathbf{z}}$-direction, the total dimension of the problem is 2, with the coordinates (z_1, z_2) denoting the positions of the particles along the $\hat{\mathbf{z}}$-axis with the centre of the pulley sitting at $z = 0$.*

Note that the potential is given by $U(z_1, z_2) = mgz_1 + mgz_2$.

Since the length of the rope is constant, we have the following constraint: $z_2 = c - z_1$, with c a constant equal to $-\ell + \pi R$, the part of the string not touching the pulley. The coordinate on our 1-dimensional submanifold $\{z_1 + z_2 - c = 0\}$ is therefore $q = z^1$. The Lagrangian on $\{z_1 + z_2 - c = 0\}$ can then be expressed as follows:

$$\mathcal{L}(q, v) = \frac{1}{2}m_1 v^2 + \frac{1}{2}m_2 v^2 - m_1 gq - m_2 g(c - q).$$

The Euler Lagrange equation is:

$$(m_1 + m_2)\ddot{q} = -(m_1 - m_2)g$$

and hence, plugging in the initial conditions gives

$$q(t) = z^1(0) - \frac{1}{2}\frac{m_1 - m_2}{m_1 + m_2} gt^2$$

for t suitably small, so that $q(t) \leq 0$ (and we do not have to deal with the string detaching from the pulley). Finally, we have that $z_2(t) = c - q(t)$.

[7] Though the actual equations of motion in Einstein's theory of gravity should still remain rather magical.

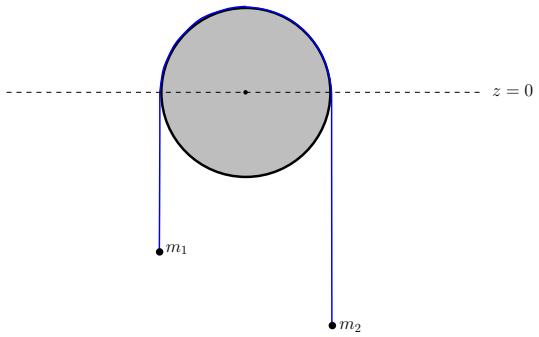

Figure 1: The Atwood machine.

Example 2.12. *Consider a free particle in* $\mathbb{R}^3$ *of mass* $m = 1$ *that is constrained to a unit round 2-sphere* $\mathbb{S}^2$*. With respect to spherical coordinates* (θ, φ)*, the induced Riemannian metric* $g \in \Gamma(T^*\mathbb{S}^2 \otimes T^*\mathbb{S}^2)$ *can be expressed as:*

$$g = d\theta^2 + \sin^2\theta d\varphi^2 = d\theta \otimes d\theta + \sin^2\theta d\varphi \otimes d\varphi.$$

The Lagrangian $\mathcal{L} : T\mathbb{S}^2 \to \mathbb{R}$ *then takes the following expression with respect to a local coordinate chart* q^i *on* $\mathbb{S}^2$*:*

$$\mathcal{L}(q, v) = \frac{1}{2} g_{ij}(q) v^i v^j.$$

The Euler–Lagrange equations give the following equation for paths $\gamma : I \to \mathbb{S}^2$ *in space*

$$\frac{1}{2}\partial_i g_{jk} \dot{\gamma}^j(t)\dot{\gamma}^k(t) - \frac{d}{dt}(g_{ij}(\gamma(t))\dot{\gamma}^j(t)) = 0.$$

By the chain rule, the above equation is equivalent to

$$0 = g_{ij}\ddot{\gamma}^j + \partial_k g_{ij}\dot{\gamma}^j\dot{\gamma}^k - \frac{1}{2}\partial_i g_{jk}\dot{\gamma}^j\dot{\gamma}^k = g_{ij}(\ddot{\gamma}^j + \Gamma^j_{mk}\dot{\gamma}^m\dot{\gamma}^k),$$

with

$$\Gamma^j_{mk} = \frac{1}{2}(g^{-1})^{jn}(\partial_m g_{kn} + \partial_k g_{mn} - \partial_n g_{mk}).$$

The numbers Γ^j_{mk} *are called the* Christoffel symbols*. They are intimately connected to* g *and we will later see them when we discuss natural notions of derivatives on manifolds equipped with metrics. We will see that these Euler–Lagrange equations are precisely the equations of an* affinely parametrized geodesic*.*

3 Lagrangian field theory

We have seen that Newton's equations, a system of ODE with solutions corresponding to paths

$$\gamma : [a, b] \to \mathbb{R}^{3N},$$

representing dynamical *particles*, can be obtained by extremizing an action of the form

$$\mathcal{S}(\gamma) = \int_a^b \mathcal{L}(t, \gamma(t), \dot{\gamma}(t))\, dt.$$

We will see that the equations of motion of *fields*, like the electric and magnetic fields, which we will interpret as tensor fields on $\mathbb{R}^{n+1}$ and on more general spacetime manifolds, can also be obtained by extremizing an action with an appropriate Lagrangian. In this case, the equations are PDE (partial differential equations) instead of ODE. Since fields are maps with as their domain spacetime regions, rather than time intervals, we need to make the following schematic form of the Lagrangian $\mathcal{L}$ precise:

$$\mathcal{L}(\text{field, derivative of field, spacetime point})$$

To be able to define this action cleanly and to be able to easily generalize to the setting of manifolds, we take a detour and introduce some geometric concepts. In particular, it is convenient to have a suitable coordinate-independent notion of the *derivative of a tensor field*.

3.1 Metrics and connections

Consider a manifold $\mathcal{M}$ equipped with $g \in \mathcal{T}^{(0,2)}(\mathcal{M}) = \Gamma(T^*\mathcal{M} \otimes T^*\mathcal{M})$, with g a symmetric, non-degenerate (0,2)-tensor field called a *metric tensor field*. We therefore have that $g : x \mapsto g_x \in T_x^*\mathcal{M} \otimes T_x^*\mathcal{M}$, with each $g_x : T_x\mathcal{M} \times T_x\mathcal{M} \to \mathbb{R}$ a bilinear map that is symmetric and non-degenerate.

Let $X, Y \in \mathcal{T}(\mathcal{M})$, with $X(x) = (x, X_x)$ and $Y(x) = (x, Y_x)$. Then we also denote $g(X, Y) \in C^\infty(\mathcal{M})$ where $g(X, Y)(x) = g_x(X_x, Y_x)$.

3.1.1 Musical isomorphisms

Via the metric tensor field, which we will refer to as a *metric*, we will obtain an isomorphism between $T_x\mathcal{M}$ and $T_x^*\mathcal{M}$ for each $x \in \mathcal{M}$. Indeed, consider the map $\flat : T\mathcal{M} \to T^*\mathcal{M}$, defined as follows:

$$\flat : (x, v) \mapsto (x, g_x(\cdot, v)),$$

where $g_x(\cdot, v) : T_x\mathcal{M} \to \mathbb{R}$ is a linear map and is therefore an element of $T_x^*\mathcal{M}$, so $\flat(x, \cdot) : T_x\mathcal{M} \to T_x^*\mathcal{M}$ is a well-defined linear map. By the non-degeneracy of g, $\ker \flat(x, \cdot) = \{0\}$, so we can apply the rank–nullity theorem to conclude that $\flat(x, \cdot)$ is in fact bijective. We denote the corresponding inverse map by $\sharp : T^*\mathcal{M} \to T\mathcal{M}$, with $\sharp(x, \cdot) = \flat(x, \cdot)^{-1}$. The maps $\flat$ and $\sharp$ are called *musical isomorphisms*.

We will also employ the same notation for maps between vector fields and 1-forms: $\flat : \mathcal{T}(\mathcal{M}) \to \Omega^1(\mathcal{M})$ and $\sharp : \Omega^1(\mathcal{M}) \to \mathcal{T}(\mathcal{M})$, with $\flat(X)(x) = \flat(X(x))$ and $\sharp(\omega)(x) = \sharp(\omega(x))$, and we denote $X^\flat := \flat(X)$ and $\omega^\sharp = \sharp(\omega)$.

We define the *inverse metric tensor field* (or inverse metric, short) $g^{-1} \in \mathcal{T}^{(2,0)}(\mathcal{M}) = \Gamma(T\mathcal{M} \otimes T\mathcal{M})$ as follows:

$$g^{-1}(\omega, \theta) = g(\sharp(\omega), \sharp(\theta)).$$

We then immediately obtain: $g(X, Y) = g^{-1}(\flat(X), \flat(Y))$ for all $X, Y \in \mathcal{T}(\mathcal{M})$. The inverse metric is a symmetric, non-degenerate $(2, 0)$-tensor field.

It is instructive to investigate the above maps with respect to a coordinate chart $(U, \{x^\mu\})$. We can then express:

$$g = g_{\mu\nu} dx^\mu dx^\nu := g_{\mu\nu} dx^\mu \otimes dx^\nu,$$

with $g_{\mu\nu} \in C^\infty(U)$. Let $X = X^\alpha \partial_{x^\alpha} \in \mathcal{T}(\mathcal{M})$ and $Y = Y^\alpha \partial_{x^\alpha} \in \mathcal{T}(\mathcal{M})$. Then we can express in U:

$$X^\flat(Y) := \flat(X)(Y) = g_{\mu\nu} X^\nu Y^\mu.$$

hence, $X^\flat = g_{\mu\nu}X^\nu dx^\mu$. In particular,

$$(\partial_{x^\beta})^\flat = g_{\mu\beta}dx^\mu.$$

We will denote the components of $X^\flat$ with an index in the subscript, i.e. $X_\mu := g_{\mu\nu}X^\nu$. For this reason, it is said that the map $\flat$, "lowers indices".

We can express in U:

$$g^{-1} = (g^{-1})^{\mu\nu}\partial_{x^\mu}\partial_{x^\nu} := (g^{-1})^{\mu\nu}\partial_{x^\mu} \otimes \partial_{x^\nu}.$$

By the definition of g^{-1}, we have that:

$$g_{\mu\nu} = g(\partial_{x^\mu}, \partial_{x^\nu}) = g^{-1}((\partial_{x^\mu})^\flat, (\partial_{x^\nu})^\flat) = g_{\mu\alpha}g_{\nu\beta}g^{-1}(dx^\alpha, dx^\beta) = g_{\mu\alpha}g_{\nu\beta}(g^{-1})^{\alpha\beta}$$

and hence

$$g_{\nu\beta}(g^{-1})^{\alpha\beta} = \delta^\alpha_\nu.$$

This means that the matrix with components $(g^{-1})^{\mu\nu}$ is the inverse of the matrix with components $g_{\mu\nu}$.

Let $\omega = \omega_\alpha dx^\alpha$ and $\theta = \theta_\alpha dx^\alpha$ be 1-forms in U. Then:

$$\omega^\sharp(\theta) := (g^{-1})^{\mu\nu}\omega_\nu\theta_\mu,$$

so $\omega^\sharp = (g^{-1})^{\mu\nu}\omega_\nu\partial_{x^\mu}$. Note that

$$\flat(\sharp(\omega)) = g_{\mu\nu}(g^{-1})^{\nu\alpha}\omega_\alpha dx^\mu = \delta^\alpha_\mu\omega_\alpha dx^\alpha = \omega_\mu dx^\mu = \omega,$$

so $\omega^\sharp = \sharp(\omega)$.

Hence, the map $\sharp$ "raises indices". We will denote the components of $\omega^\sharp$ with an index in the superscript, i.e. $\omega^\mu := (g^{-1})^{\mu\nu}\omega_\nu$.

Comment on index placement: When applying the Einstein summation convention with repeated indices, it is convention to place one index in the superscript and one index in the subscript. Components of a vector field X with respect to a basis are denoted with X^μ and the coordinate basis vector fields are denoted with ∂_{x^μ} or ∂_μ, so that X can be expressed locally as the sum $X^\mu\partial_\mu$. Similarly, components of a 1-form ω are denoted with ω_μ and the basis of 1-forms dual to ∂_{x^μ} is denoted with dx^μ, so that $\omega = \omega_\mu dx^\mu$.

By identifying the bilinear maps $g_x : T_x\mathcal{M} \times T_x\mathcal{M} \to \mathbb{R}$ with symmetric matrices with coefficients $g_x(e_\mu, e_\nu)$ with respect to a basis $\{e_0, \ldots, e_n\}$, we can investigate the corresponding eigenvalues. These eigenvalues are non-zero, by the non-degeneracy assumption. The number of positive and negative eigenvalues of $g_x : T_x\mathcal{M} \times T_x\mathcal{M} \to \mathbb{R}$ corresponds to the maximal dimensions of the subspaces on which g_x is positive-definite or negative-definite, respectively. These spaces are independent of the basis we chose on $T_x\mathcal{M}$; this is known as *Sylvester's Law of Inertia.*[8]

By the symmetry of g_x, there always exist a basis $\{e_0, \ldots, e_n\}$ in which the matrix representing g_x is diagonal. We can moreover rescale the basis vectors so that $g(e_\mu, e_\nu) = \pm 1$. Such a basis is called an *orthonormal basis*. The corresponding matrix is diagonal with $+1$ or -1 as its entries and the number of $+1$ and -1 is independent of choice of orthonormal basis, as it corresponds to the number of positive and negative eigenvalues, respectively.

If the number of positive and negative eigenvalues is independent of $x \in \mathcal{M}$,[9] we can define the *signature* of a metric tensor field as the pair (p, n) with p the total number of positive eigenvalues and n the total number of negative eigenvalues. Alternatively, the signature can be represented by a list of numbers $+1$ or -1. A Riemannian metric tensor field then has signature $(+\ldots+)$ (all positive eigenvalues) at each point in the manifold. We will refer to these metric tensor fields as "Riemannian metrics" and the pairing $(\mathcal{M}, g)$ as a Riemannian manifold.

[8] Sylvester's Law of Inertia says that if A is an $n \times n$ symmetric matrix with n_+ positive eigenvalues and n_- negative eigenvalues, then, for any $n \times n$ matrix B, the symmetric matrix BAB^T will also have n_+ positive eigenvalues and n_- negative eigenvalues. If A denotes the matrix with coefficients $g_x(e_\mu, e_\nu)$, then a change of basis on the tangent space, given by $f_\mu = B_{\mu\alpha}e_\alpha$ will lead to a matrix C with coefficients $g_x(f_\mu, f_\nu)$. We have that $C = BAB^T$.

[9] Exercise: Convince yourself that the number of positive and negative eigenvalues is always constant on each connected component of $\mathcal{M}$.

Definition 3.1. *We define a* Lorentzian metric tensor field *to be a metric tensor field with signature* $(-+\ldots+)$ *(one negative eigenvalue and n positive eigenvalues) at each point in the manifold. We will refer to these metric tensor fields as "Lorentzian metrics". Metric tensor fields with more general signatures are referred to as* pseudo-Riemannian metrics.

We refer to the corresponding manifolds $(\mathcal{M}, g)$ *with* g *a Lorentzian metric as a* Lorentzian manifold.

3.1.2 The Levi–Civita connection

Before we can introduce Lagrangians and actions, we will need to make sense of a notion of derivative that is compatible with the structure g.

Definition 3.2. *An* affine connection *is a bilinear map* $\nabla : \mathcal{T}(\mathcal{M}) \times \mathcal{T}(\mathcal{M}) \to \mathcal{T}(\mathcal{M})$ *with* $(X, Y) \mapsto \nabla_X Y$*, such that for all* $X, Y \in \mathcal{T}(\mathcal{M})$ *and* $f \in C^\infty(\mathcal{M})$

1. *(linearity over* $C^\infty(\mathcal{M})$*)* $\nabla_{fX} Y = f \nabla_X Y$*,*
2. *(Leibniz rule)* $\nabla_X (fY) = X(f)Y + f\nabla_X Y$*.*

An affine connection is a Levi-Civita connection *with respect to a pseudo-Riemannian metric* g *if for all* $X, Y, Z \in \mathcal{T}(\mathcal{M})$*:*

1. *(metric-preserving)* $X(g(Y, Z)) = g(\nabla_X Y, Z) + g(Y, \nabla_X Z)$*,*
2. *(torsion free)* $\nabla_X Y - \nabla_Y X = [X, Y]$*.*

We define the *covariant derivative* as the map:

$$\begin{aligned} \nabla : \mathcal{T}(\mathcal{M}) &\to \mathcal{T}^{(1,1)}(\mathcal{M}), \\ (\nabla Y)(X, \omega) &:= \omega(\nabla_X Y). \end{aligned}$$

with $\mathcal{T}^{(1,1)}(\mathcal{M})$ the space of $(1,1)$-tensor fields. Recall that an smooth (r,s)-tensor field $T \in \mathcal{T}^{(r,s)}\mathcal{M} = \Gamma(\underbrace{T\mathcal{M} \otimes \ldots T\mathcal{M}}_{r \text{ times}} \otimes \underbrace{T^*\mathcal{M} \otimes \ldots T^*\mathcal{M}}_{s \text{ times}})$.

Note that ∇Y is a well-defined tensor field because it is bilinear over $C^\infty(\mathcal{M})$. Exercise: Verify this by considering $(\nabla Y)(fX + Z, h\omega + \alpha)$ for $f, h \in C^\infty(\mathcal{M})$, $X, Y, Z \in \mathcal{T}(\mathcal{M})$ and $\omega, \alpha \in \Omega^1(\mathcal{M})$.

Theorem 3.1. *Let* $(\mathcal{M}, g)$ *be a pseudo-Riemannian manifold. Then there exists a unique Levi–Civita connection with respect to* g*.*

Proof. We will first prove uniqueness. Let $X, Y, Z \in \mathcal{T}(M)$. By the metric preserving property and symmetry of g, we have that

$$X(g(Y,Z)) + Y(g(Z,X)) - Z(g(Y,X)) = g(\nabla_X Y + \nabla_Y X, Z) + g(\nabla_X Z - \nabla_Z X, Y) + g(\nabla_Y Z - \nabla_Z Y, X).$$

Applying the torsion free condition then gives

$$X(g(Y,Z)) + Y(g(Z,X)) - Z(g(Y,X)) = 2g(\nabla_X Y, Z) - g([X,Y],Z) + g([X,Z],Y) + g([Y,Z],X).$$

Rearranging terms then gives

$$g(\nabla_X Y, Z) = \frac{1}{2}\left(X(g(Y,Z)) + Y(g(Z,X)) - Z(g(Y,X)) + g([X,Y],Z) - g([X,Z],Y) - g([Y,Z],X)\right). \tag{3.1}$$

Suppose there exists another Levi-Civita connection $\widetilde{\nabla}$, then by the linearity of g

$$g(\nabla_X Y - \widetilde{\nabla}_X Y, Z) = 0$$

for all $X, Y, Z \in \mathcal{T}(\mathcal{M})$. By the non-degeneracy of g, this must mean that $\nabla_X Y - \widetilde{\nabla}_X Y = 0$ for all $X, Y \in \mathcal{T}(\mathcal{M})$.

We can similarly use (3.1) to prove the existence of ∇. Indeed, we have that $(\nabla_X Y)^\flat \in \Omega^1(\mathcal{M})$ can be defined as follows: let $X, Y, Z \in \mathcal{T}(M)$, then

$$(\nabla_X Y)^\flat(Z) := \frac{1}{2}\left(X(g(Y,Z)) + Y(g(Z,X)) - Z(g(Y,X)) + g([X,Y],Z) - g([X,Z],Y) - g([Y,Z],X)\right).$$

Indeed, $(\nabla_X Y)^\flat$ is a well-defined 1-form by linearity of the right-hand side above in Z. We leave it as an Exercise to verify that $(X,Y) \mapsto (\nabla_X Y) := \sharp((\nabla_X Y)^\flat)$ defines a Levi-Civita connection. □

We can express the Levi–Civita connection as follows with respect to a coordinate chart $\{x^\mu\}$:

$$(\nabla_{\partial_\mu}\partial_\nu)^\sigma = \frac{1}{2}(g^{-1})^{\sigma\rho}\left(\partial_\mu g_{\nu\rho} + \partial_\nu g_{\mu\rho} - \partial_\rho g_{\mu\nu}\right) =: \Gamma^\sigma_{\mu\nu}.$$

The expressions $\Gamma^\sigma_{\mu\nu}$ are called the Christoffel symbols. Hence,

$$\begin{aligned}(\nabla_X Y)^\sigma &= (\nabla_{X^\mu\partial_\mu}(Y^\nu\partial_\nu))^\sigma = X^\mu\partial_\mu Y^\sigma + \Gamma^\sigma_{\mu\nu}X^\mu Y^\nu,\\ (\nabla Y)^\sigma{}_\mu &= \partial_\mu Y^\sigma + \Gamma^\sigma_{\mu\nu}Y^\nu.\end{aligned}$$

We would like to extend ∇ to act on more general tensor fields: $\nabla : \mathcal{T}^{(r,s)}(\mathcal{M}) \to \mathcal{T}^{(r,s+1)}(\mathcal{M})$. First, we let $\nabla f := df$ for $f \in C^\infty(\mathcal{M}) = T^{(0,0)}(\mathcal{M})$. This implies that $C^\infty(\mathcal{M}) \ni \nabla_X f = df(X) = X(f)$.

Next, we consider $\omega \in \Omega^1(\mathcal{M}) = \mathcal{T}^{(0,1)}(\mathcal{M})$ and define

$$(\nabla\omega)(X,Y) := \nabla_X(\omega(Y)) - \omega(\nabla_X Y)$$

for all $Y, Z \in \mathcal{T}(\mathcal{M})$. Note that linearity over $C^\infty(\mathcal{M})$ in the first argument follows immediately, and linearity in the second argument follows from:

$$(\nabla\omega)(X,fY) = \nabla_X(\omega(fY)) - \omega(\nabla_X(fY)) = f(\nabla\omega)(X,Y) + (\nabla_X f)\omega(Y) - (\nabla_X f)\omega(Y) = f(\nabla\omega)(X,Y).$$

This definition ensures that ∇ is compatible with tensor contraction. With respect to a coordinate chart $(U, \{x^\mu\})$, we obtain for all $0 \le \nu \le n+1$

$$\nabla_\nu(\omega_\rho Y^\rho) = (\nabla\omega)_{\nu\rho}Y^\rho + \omega_\rho(\nabla Y)^\rho{}_\nu.$$

We can therefore also express:

$$(\nabla\omega)_{\nu\mu} = \partial_\nu\omega_\mu - \Gamma^\rho_{\mu\nu}\omega_\rho.$$

We will use the following notational conventions:

$$\begin{aligned}\nabla_\nu\omega_\mu &:= (\nabla\omega)_{\nu\mu},\\ \nabla_\nu Y^\mu &:= (\nabla Y)^\mu{}_\nu\end{aligned}$$

We now extend ∇ as a map on general tensor fields: $\nabla : \mathcal{T}^{(r,s)}(\mathcal{M}) \to \mathcal{T}^{(r,s+1)}(\mathcal{M})$ by making it compatible with tensor contraction.

For $T \in \mathcal{T}^{(r,s)}(\mathcal{M})$, we define:

$$\begin{aligned}(\nabla_X T)(\omega_1,\dots,\omega_r,Y_1,\dots,Y_s) &= X(T(\omega_1,\dots,\omega_r,Y_1,\dots,Y_s))\\ &\quad - T(\nabla_X\omega_1,\dots,\omega_r,Y_1,\dots,Y_s) - \dots - T(\nabla_X\omega_1,\dots,\nabla_X\omega_r,Y_1,\dots,Y_s)\\ &\quad - T(\omega_1,\dots,\omega_r,\nabla_X Y_1,\dots,Y_s) - \dots - T(\omega_1,\dots,\omega_r,Y_1,\dots,\nabla_X Y_s).\end{aligned}$$

A tensor field T takes the following form with respect to a coordinate chat $(U, \{x^\mu\})$:

$$T = T^{\nu_1\dots\nu_r}{}_{\mu_1\dots\mu_s}\partial_{x^{\nu_1}} \otimes \dots \otimes \partial_{x^{\nu_r}} \otimes dx^{\mu_1} \otimes dx^{\mu_s},$$

with $T^{\nu_1\dots\nu_r}{}_{\mu_1\dots\mu_s} \in C^\infty(\mathcal{M})$ smooth functions. In the notation, we do not put the upper and lower indices directly above each other, so that we can lower and raise them using the musical isomorphisms.

We then obtain:

$$\begin{aligned}\nabla_\mu T^{\nu_1\dots\nu_r}{}_{\mu_1\dots\mu_s} &= \partial_\mu T^{\nu_1\dots\nu_r}{}_{\mu_1\dots\mu_s} - \Gamma^\rho_{\mu\mu_1}T^{\nu_1\dots\nu_r}{}_{\rho\dots\mu_s} - \Gamma^\rho_{\mu\mu_2}T^{\nu_1\dots\nu_r}{}_{\mu_1\rho\mu_3\dots\mu_s} - \dots - \Gamma^\rho_{\mu\mu_s}T^{\nu_1\dots\nu_r}{}_{\mu_1\dots\mu_{s-1}\rho}\\ &\quad + \Gamma^{\nu_1}_{\mu\rho}T^{\rho\nu_2\dots\nu_r}{}_{\mu_1\dots\mu_s} + \Gamma^{\nu_2}_{\mu\rho}T^{\nu_1\rho\nu_3\dots\nu_r}{}_{\mu_1\dots\mu_s} + \dots + \Gamma^{\nu_r}_{\mu\rho}T^{\nu_1\dots\nu_{r-1}\rho}{}_{\mu_1\dots\mu_s}.\end{aligned}$$

By construction, we have in particular that $\nabla g = 0$.

3.1.3 The natural volume form and Hodge dual

It will be useful to derive a divergence theorem involving ∇. To make sense of that, we first need a natural way of integrating on $(\mathcal{M}, g)$. We will need assume that $\mathcal{M}$ is *oriented*. This means that there exists a global volume form ω that is non-vanishing everywhere. A coordinate chart $(U, \{x^\mu\})$ is said to be *positively oriented* if $\omega = f dx^0 \wedge \ldots \wedge dx^n$, with f a positive function on U. We say a (local) basis of vector fields $(E_0, \ldots, E_n)$ is *positively oriented* if $\omega(E_0, \ldots, E_n) > 0$.

Lemma 3.2. *Let $(\mathcal{M}, g)$ be an n-dimensional oriented pseudo-Riemannian manifold. Then there exists a unique volume form ϵ, which satisfies the property that*

$$\epsilon(E_0, \ldots, E_n) = 1$$

for any positively oriented, local basis of orthonormal vector fields $E_0, \ldots, E_n$.

With respect to a positively oriented coordinate chart $(U, \{x^\mu\})$, ϵ can be expressed as follows:

$$\epsilon = \sqrt{|\det g|} dx^0 \wedge \ldots \wedge dx^n.$$

Proof. Exercise. □

Definition 3.3. *Let $n \in \mathbb{N}$ and $r \leq n$. Let $(\mathcal{M}, g)$ be an n-dimensional, oriented pseudo-Riemannian manifold. The* Hodge dual *is a map*

$$\star : \Omega^r(\mathcal{M}) \to \Omega^{n-r}(\mathcal{M}),$$

with $(\star\omega) := \star(\omega)$, that is linear over $C^\infty(\mathcal{M})$, i.e. for all $\omega, \alpha \in \Omega^r(\mathcal{M})$ and $f \in C^\infty(\mathcal{M})$

$$\star(f\omega + \alpha) = f \star \omega + \star\alpha,$$

and for $\omega = \omega^1 \wedge \ldots \wedge \omega^r \in \Omega^r(\mathcal{M})$,

$$(\star\omega)(X_1, \ldots, X_{n-r}) = \epsilon(X_1, \ldots, X_{n-r}, \omega_1^\sharp, \ldots, \omega_r^\sharp).$$[10]

With respect to a coordinate chart $(U, \{x^\mu\})$, we can express:

$$(\star\omega)_{\mu_1 \ldots \mu_{n-r}} = \frac{1}{r!} \epsilon_{\mu_1 \ldots \mu_n} \omega^{\mu_{n-r+1} \cdots \mu_n},$$

where the $r!$ factor arises from:

$$\omega = \omega_{\mu_1 \ldots \mu_r} dx^{\mu_1} \otimes \ldots \otimes dx^{\mu_r} = \frac{1}{r!} \omega_{\mu_1 \ldots \mu_r} dx^{\mu_1} \wedge \ldots \wedge dx^{\mu_r}.$$

Lemma 3.3. (i) *The following identity holds:*

$$\epsilon_{\mu_1 \ldots \mu_n} \epsilon^{\nu_1 \ldots \nu_r \mu_{n-r} \cdots \mu_n} = \operatorname{sign}(\det g) r!(n-r)! \delta^{\nu_1}_{[\mu_1} \ldots \delta^{\nu_r}_{\mu_r]},$$

where square brackets denote the antisymmetrization of the indices, i.e.

$$A_{[\mu_1 \ldots, \mu_r]} = \frac{1}{r!} \sum_{\sigma \in S(\{\mu_1, \ldots, \mu_r\})} \operatorname{sign}(\sigma) A_{\sigma(\mu_1) \ldots, \sigma(\mu_r)},$$

with $S(\{\mu_1, \ldots, \mu_r\})$ the set of all permutations of $\{\mu_1, \ldots, \mu_r\}$.

(ii) *Let $\omega \in \Omega^r(\mathcal{M})$, then*

$$\star(\star\omega) = \operatorname{sign}(\det g)(-1)^{r(n-r)} \omega,$$

where the sign corresponds to the sign of $\det g$.

[10] Exercise: Convince yourself that for $\omega \in \Omega^r(\mathcal{M})$, $\star\omega$ is globally well-defined on $\mathcal{M}$.

(iii) *Let $\omega \in \Omega^r(\mathcal{M})$, then*

$$\star(d\star\omega)_{\mu_1\dots\mu_{r-1}} = \operatorname{sign}(\det g)(-1)^{r(n-r)}\nabla^{\mu_r}\omega_{\mu_1\dots\mu_r},$$

where the sign corresponds to the sign of $\det g$ *and* ∇_μ *is taken with respect to an arbitrary choice of coordinate chart.*

Proof. Problem sheet. □

Lemma 3.4. $\nabla\epsilon = 0$

Proof. By (i) of Lemma 3.3, we have that in the domain of a coordinate chart:

$$\nabla_\nu(\epsilon_{\mu_0\dots\mu_n}\epsilon^{\mu_0\cdots\mu_n}) = \nabla_\nu(\operatorname{sign}(\det g)n!) = 0.$$

Furthermore, by $\nabla g = 0$ and the compatibility of ∇ with contraction, we can express

$$\nabla_\nu(\epsilon_{\mu_0\dots\mu_n}\epsilon^{\mu_0\cdots\mu_n}) = (\nabla_\nu\epsilon_{\mu_0\dots\mu_n})\epsilon^{\mu_0\cdots\mu_n} + \epsilon_{\mu_0\dots\mu_n}(\nabla_\nu\epsilon^{\mu_0\cdots\mu_n}) = 2\epsilon^{\mu_0\cdots\mu_n}\nabla_\nu\epsilon_{\mu_0\dots\mu_n}.$$

Finally, note that by the antisymmetry properties of ϵ

$$\epsilon^{\mu_0\cdots\mu_n}\nabla_\nu\epsilon_{\mu_0\dots\mu_n} = n!\epsilon^{0\dots n}\nabla_\nu\epsilon_{0\dots n}.$$

Since $\epsilon^{0\dots n} \neq 0$, we must have that $\nabla_\nu\epsilon_{0\dots n}$ vanishes, so, by the antisymmetry of ϵ, $\nabla_\nu\epsilon_{0\dots n} = 0$ for all ν and $\nabla\epsilon = 0$. □

Proposition 3.5. *Let $(\mathcal{M}, g)$ be an n-dimensional, oriented, pseudo-Riemannian manifold-with-boundary and let $X \in \mathcal{T}(\mathcal{M})$. Then*

$$\int_{\mathcal{M}} \nabla_\mu X^\mu \,\epsilon = (-1)^{n-1}\int_{\partial\mathcal{M}} \iota^*(\star X^\flat),$$

where $\iota : \partial\mathcal{M} \to \mathcal{M}$ is the inclusion map.

Proof. Consider $X^\flat \in \Omega^1(\mathcal{M})$. Then $\star X^\flat \in \Omega^{n-1}(\mathcal{M})$. By (iii) and (ii) of Lemma 3.3, we have that

$$(\nabla_\mu X^\mu)\epsilon = \star(\nabla^\mu X_\mu) = \star(\operatorname{sign}(\det g)(-1)^{n-1}\star(d\star X^\flat)) = (-1)^{n-1}d\star X^\flat.$$

By Stokes' theorem, we have that

$$\int_{\mathcal{M}}(-1)^{n-1}d\star X^\flat = (-1)^{n-1}\int_{\partial\mathcal{M}}\iota^*(\star X^\flat).$$ □

Given a vector field $X \in \mathcal{T}(\mathcal{M})$, we will denote with $\operatorname{div} X$ the function in $C^\infty(\mathcal{M})$ that takes the form $\nabla_\mu X^\mu$ locally with respect to an arbitrary coordinate chart.

3.2 Lagrangian field theory

Let $(\mathcal{M}, g)$ be an $n+1$-dimensional, orientable, pseudo-Riemannian manifold(-with-boundary). We define the *field manifold* $\mathcal{N}$ as the disjoint union:

$$\mathcal{N} = \coprod_{x\in\mathcal{M}} \wedge^r T^*_x\mathcal{M} \times (T^*_x\mathcal{M} \otimes \wedge^r T^*_x\mathcal{M}) = \bigcup_{x\in\mathcal{M}} \{x\} \times \wedge^r T^*_x\mathcal{M} \times (T^*_x\mathcal{M} \otimes \wedge^r T^*_x\mathcal{M})$$

with projection map $\pi : \mathcal{N} \to \mathcal{M}$, $\pi(x, q, v) = x$ for $q \in \wedge^r T^*_x\mathcal{M}$ and $v \in T^*_x\mathcal{M}\otimes\wedge^r T^*_x\mathcal{M}$. Analogously to the construction of the tangent and cotangent bundle, it can be shown that given a coordinate chart $(U, \{x^\mu\})$ on $\mathcal{M}$, the pair $(\pi^{-1}(U), \tilde{\psi})$ defines a coordinate chart on $\mathcal{N}$, if we take $\tilde{\psi}(x, q, v) = (x^\mu, q_{\mu_1\dots\mu_r}, v_{\nu_1\dots\nu_{r+1}})$, where

$$q = \frac{1}{r!}q_{\mu_1\dots\mu_r}(dx^{\mu_1}\wedge\dots\wedge dx^{\mu_r})_x \in \wedge^r T^*_x U,$$

$$v = \frac{1}{r!} v_{\nu_1 \dots \nu_{r+1}} dx^{\nu_1}_x \otimes (dx^{\nu_2} \wedge \dots \wedge dx^{\nu_{r+1}})_x \in T^*_x U \otimes \wedge^r T^*_x U.$$

In this way $\mathcal{N}$ is indeed a manifold. We will moreover apply the convention $\Lambda^0 T^*\mathcal{M} = \mathbb{R}$.

We introduce the field Lagrangian as the smooth map:

$$\mathcal{L} : \mathcal{N} \to \mathbb{R}.$$

Note that $d\mathcal{L} \in \Omega^1(\mathcal{N})$ takes the following form on $\pi^{-1}(U)$:

$$d\mathcal{L} = \frac{\partial \mathcal{L}}{\partial x^\mu} dx^\mu + \frac{\partial \mathcal{L}}{\partial q^{\mu_1 \dots \mu_r}} dq^{\mu_1 \dots \mu_r} + \frac{\partial \mathcal{L}}{\partial v^{\nu_1 \dots \nu_{r+1}}} dv^{\nu_1 \dots \nu_{r+1}}.$$

We will refer to sections $\phi \in \Gamma(\wedge^r T^*\mathcal{M}) = \Omega^r(\mathcal{M})$ as *fields*. Note that $\nabla\phi \in \Gamma(T^*\mathcal{M} \otimes \wedge^r T^*\mathcal{M})$.

Let $\mathcal{M}$ be a compact manifold(with-boundary). We can then define the action $\mathcal{S} : \Omega^r(\mathcal{M}) \to \mathbb{R}$ as the following integral:

$$\mathcal{S}(\phi) = \int_{\mathcal{M}} \mathcal{L} \circ (\phi, \nabla\phi)\, \epsilon.$$

Note that $\mathcal{L} \circ (\phi, \nabla\phi) : \mathcal{M} \to \mathbb{R}$ is smooth.[11]

Exercise: Convince yourself that the above notions can easily be extended to the setting where the fields are general tensor fields, rather than differential forms.

Just like in the case of Lagrangians with domain $T(\mathbb{R} \times \mathcal{M})$, we can extremize the action and obtain Euler–Lagrange equations.

Definition 3.4. *Let $U \subset V \subseteq \mathcal{M}$ be open, with V compact, and $\mathcal{M}$ a manifold(-with-boundary). We say $\phi \in \Omega^r(U)$ is an extremal of the action $\mathcal{S} : \Omega^r(U) \to \mathbb{R}$ if for any $h \in \Omega^r(U)$, such that $h|_{\partial U} = 0$ if $\partial U \neq \emptyset$,*

$$\frac{d}{ds}\Big|_{s=0} \mathcal{S}(\phi + sh) = 0.$$

Proposition 3.6. *Consider a coordinate chart $(U, \{x^\mu\})$ on $\mathcal{M}$, such that $U \subseteq V$, with V compact. Then $\phi \in \Omega^r(U)$ is an extremal of the action $\mathcal{S} : \Omega^r(U) \to \mathbb{R}$ if and only if ϕ satisfies the following equations on U: for all $1 \leq \nu_i \leq n+1$,*

$$\frac{\partial \mathcal{L}}{\partial q_{\nu_1 \dots \nu_r}} \circ (\phi, \nabla\phi) - \nabla_\nu \left(\frac{\partial \mathcal{L}}{\partial v_{\nu\nu_1 \dots \nu_r}} \circ (\phi, \nabla\phi) \right) = 0. \tag{3.2}$$

Proof. Consider

$$\mathcal{L} : \pi^{-1}(U) \to \mathbb{R},$$

with $\pi : \mathcal{N} \to \mathcal{M}$. Let $h \in \Omega^r(U)$, such that $h|_{\partial U} = 0$. Then:

$$\begin{aligned}
\frac{d}{ds}|_{s=0} \mathcal{S}(\phi + sh) &= \int_U \frac{d}{ds}|_{s=0} \mathcal{L}(\phi(x) + sh(x), \nabla\phi(x) + s\nabla h(x))\epsilon \\
&= \int_U \frac{\partial \mathcal{L}}{\partial q_{\nu_1 \dots \nu_r}}(\phi(x), \nabla\phi(x)) h_{\nu_1 \dots \nu_r}(x) + \frac{\partial \mathcal{L}}{\partial v_{\nu\nu_1 \dots \nu_r}}(\phi(x), \nabla\phi(x)) \nabla_\nu h_{\nu_1 \dots \mu_r}(x)\, \epsilon \\
&= \int_U \left[\frac{\partial \mathcal{L}}{\partial q_{\nu_1 \dots \nu_r}}(\phi(x), \nabla\phi(x)) - \nabla_\nu \left(\frac{\partial \mathcal{L}}{\partial v_{\nu\nu_1 \dots \nu_r}} \circ (\phi, \nabla\phi) \right)(x) \right] h_{\nu_1 \dots \mu_r}(x)\, \epsilon \\
&\qquad + o(1), \qquad (3.3)
\end{aligned}$$

where we arrived at the final inequality by using that

$$\int_U (\nabla_\nu J^\nu)\epsilon = 0$$

by Proposition 3.5 and the fact that J vanishes at ∂U by $h|_{\partial U} = 0$.

Since h was arbitrary, we arrive at (3.9) by applying Lemma 2.13. □

[11] In how we express our disjoint unions of tensor spaces, $\phi(x)$ is technically a pair in $\wedge^r T^*\mathcal{M}$ consisting of the point x and an element of $\wedge^r T^*_x\mathcal{M}$, rather than just an element of $\wedge^r T^*_x\mathcal{M}$, but we will be a sloppy with this and frequently identify $\phi(x)$ with just the element in $\wedge^r T^*_x\mathcal{M}$, for the sake of convenience.

Example 3.1 (Klein–Gordon equation)**.** *Let $\mathcal{M} = \mathbb{R}^{n+1}$ and $r = 0$. Then $\mathcal{N} \cong \mathbb{R}^{n+1} \times \mathbb{R} \times \mathbb{R}^{n+1}$. Let $\{x^\mu\}$ be Cartesian coordinates. Consider $m = m_{\mu\nu} dx^\mu \otimes dx^\nu$, with $m_{00} = -1$, $m_{0i} = 0$ and $m_{ij} = \delta_{ij}$. The Lorentzian metric m is known as the Minkowski metric. Consider*

$$\mathcal{L} : \mathcal{N} \to \mathbb{R}, \quad \text{with}$$
$$\mathcal{L}(x, q, v) = \frac{1}{2} m_x^{-1}(v, v) + \frac{\mathfrak{m}^2}{2} q^2,$$

with $\mathfrak{m} \in \mathbb{R}$. Then $\mathcal{L}(\phi(x), \nabla\phi(x)) = \frac{1}{2} m_x^{-1}(\nabla\phi(x), \nabla\phi(x)) + \frac{\mathfrak{m}^2}{2}\phi^2(x)$.

We have that

$$\frac{\partial \mathcal{L}}{\partial q}(\phi(x), \nabla\phi(x)) = \mathfrak{m}^2 \phi(x),$$
$$\nabla_\mu \left(\frac{\partial \mathcal{L}}{\partial v_\mu} \circ (\phi, \nabla\phi) \right)(x) = \nabla_\mu \nabla^\mu \phi(x).$$

The Euler–Lagrange equations therefore imply that

$$\nabla_\mu \nabla^\mu \phi = \mathfrak{m}^2 \phi,$$

We denote $\Box_g \phi := \nabla_\mu \nabla^\mu \phi$, with ∇ the Levi-Civita connection corresponding to g.

Note that in Cartesian coordinates, $\Gamma^\mu_{\nu\rho} = 0$, so $\Box_m \phi = -\partial^2_{x^0}\phi + \sum_{i=1}^n \partial^2_{x^i}\phi$ so with $t = x^0$

$$-\partial_t^2 \phi + \sum_{i=1}^n \partial_i^2 \phi = \mathfrak{m}^2 \phi,$$

which is the Klein–Gordon equation with mass $\mathfrak{m}$. The $\mathfrak{m} = 0$ case is called the (massless) wave equation.

Example 3.2 (Maxwell equations in vacuum)**.** *Let $\mathcal{M} = \mathbb{R}^{3+1}$ and $r = 1$ and let $\{x^\mu\}$ be Cartesian coordinates. Consider $(\mathbb{R}^{3+1}, m)$. Denote with m the Minkowski metric on $\mathbb{R}^{3+1}$. We define:*

$$\mathcal{L} : \mathcal{N} \to \mathbb{R}, \quad \text{with}$$
$$\mathcal{L}(x, q, v) = -\frac{1}{4}(m^{-1})^{\alpha\mu}_x (m^{-1})^{\beta\nu}_x (v_{\mu\nu} - v_{\nu\mu})(v_{\alpha\beta} - v_{\beta\alpha}).$$

Consider the field $A \in \Omega^1(\mathcal{M})$ with covariant derivative $\nabla A \in \Gamma(T^*\mathcal{M} \otimes \wedge^1 T^*\mathcal{M})$.

Then

$$\mathcal{L}((A, \nabla A)(x)) = -\frac{1}{4}(m^{-1})^{\alpha\gamma}(m^{-1})^{\beta\delta}(\nabla_\alpha A_\beta - \nabla_\beta A_\alpha)(\nabla_\gamma A_\delta - \nabla_\delta A_\gamma)(x).$$

We have that

$$\frac{\partial \mathcal{L}}{\partial q_\mu} \circ (A, \nabla A) = 0,$$
$$\nabla_\mu \left(\frac{\partial \mathcal{L}}{\partial v_{\mu\nu}} \circ (A, \nabla A) \right) = -\nabla_\mu(\nabla^\mu A^\nu - \nabla^\mu A^\nu) = -\nabla_\mu F^{\mu\nu},$$

with $F = dA$. Indeed,

$$F = \frac{1}{2}(\partial_\mu A_\nu - \partial_\nu A_\mu) dx^\mu \wedge dx^\nu = (\partial_\mu A_\nu - \partial_\nu A_\mu) dx^\mu \otimes dx^\nu = (\nabla_\mu A_\nu - \nabla_\nu A_\mu) dx^\mu \otimes dx^\nu.$$

Using F, the Lagrangian takes the form

$$\mathcal{L} \circ (A, \nabla A) = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu}.$$

By (iii) *of Lemma 3.3, we can put the Euler–Lagrange equations in the following form:*

$$dF = 0,$$

$$d \star F = 0.$$

Note that F has $\binom{4}{2} = 6$ independent components when expanded in a coordinate basis. Let us denote $\mathbf{E} = (F_{01}, F_{02}, F_{03})^T$ and $\mathbf{B} = (-F_{23}, -F_{31}, -F_{12})^T$, i.e. $E_i = F_{0i}$ and $B_i = \frac{1}{2}\epsilon_{ijk}F^{jk}$. Then the equation $dF = 0$ implies that

$$\partial_{[\mu} F_{\nu\rho]} = 0.$$

Using moreover the antisymmetry of $F_{\mu\nu}$ in its indices, we obtain: for all $0 \leq \mu, \nu, \rho \leq n$

$$\partial_\mu F_{\nu\rho} + \partial_\nu F_{\rho\mu} + \partial_\rho F_{\mu\nu} = 0$$

Note that this gives four independent equations, with $(\mu, \nu, \rho) = \{(0,1,2), (0,1,3), (0,2,3), (1,2,3)\}$. One can verify that the first three choices result in the equation:

$$\partial_t \mathbf{B} + \nabla \times \mathbf{E} = 0. \tag{3.4}$$

The final choice results in

$$\operatorname{div} \mathbf{B} = 0. \tag{3.5}$$

The equation $\nabla_\nu F^{\mu\nu}$ gives four equations. The case $\mu = 0$ results in

$$\operatorname{div} \mathbf{E} = 0 \tag{3.6}$$

and $1 \leq \mu \leq 3$ give

$$\partial_t \mathbf{E} - \nabla \times \mathbf{B} = 0. \tag{3.7}$$

The equations (3.4)–(3.7) are the Maxwell equations in vacuum and F is called the Faraday tensor*.*

Example 3.3 (Minimal surface equation)**.** *Let $\mathcal{M} = \Omega \subseteq \mathbb{R}^2$ be compact, $r = 0$ and let e be the Euclidean metric on $\mathbb{R}^2$. Then $\mathcal{N} \cong \Omega \times \mathbb{R} \times \mathbb{R}^2$. Consider*

$$\begin{aligned} \mathcal{L} &: \mathcal{N} \to \mathbb{R}, \\ \mathcal{L}(x, q, v) &= \sqrt{1 + e_x^{-1}(v, v)}. \end{aligned}$$

Then, for $u \in C^\infty(\Omega)$, $\nabla u \in \Omega^1(\Omega)$,

$$\mathcal{L}((u, \nabla u)(x)) = \sqrt{1 + |\nabla u|^2}(x).$$

We therefore have that

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial q} \circ (u, \nabla u)(x) &= 0, \\ \nabla_i \left(\frac{\partial \mathcal{L}}{\partial v_i} \circ (u, \nabla u) \right)(x) &= \nabla_i \left(\frac{\nabla^i u}{\sqrt{1 + |\nabla u|^2}} \right)(x). \end{aligned}$$

The Euler–Lagrange equations in the interior of Ω are therefore:

$$\nabla_i \left(\frac{\nabla^i u}{\sqrt{1 + |\nabla u|^2}} \right) = 0. \tag{3.8}$$

The graph $S = \{(x, u(x)) \in \mathbb{R}^3 \,|\, x \in \Omega\}$ is a 2-surface with boundary $u(\partial\Omega) \subset \mathbb{R}^3$ and the action $\mathcal{S}(u)$ gives the area of the surface. Extremals of the action can therefore be associated to surfaces with boundary $u(\partial\Omega)$ that extremize the area. It can be shown that the extremals are local minimizers of the action. The equation (3.8) is therefore called the minimal surface equation*. Note that the above discussion does not tell us anything about the existence of minimal surfaces.*

3.3 Noether's theorem

We will now investigate the relation between symmetries of actions and Lagrangians with the existence of conservation laws. In this section, we will slightly generalize our notion of Lagrangian in order to incorporate vector-valued fields. Let V be some fixed, m-dimensional vector space. We define

$$\mathcal{N} = \coprod_{x\in\mathcal{M}} (\wedge^r T_x^*\mathcal{M}\otimes V)\times(T_x^*\mathcal{M}\otimes\wedge_x^r T^*\mathcal{M}\otimes V)$$

with projection map $\pi:\mathcal{N}\to\mathcal{M}$, $\pi(x,q,v)=x$ for $q\in\wedge^r T_x^*\mathcal{M}\otimes V$ and $v\in\wedge_x^r T^*\mathcal{M}\otimes T_x^*\mathcal{M}\otimes V$. The coordinate chart on $\pi^{-1}(U)$ associated to a coordinate chart $\{x^\mu\}$ on $U\subseteq\mathcal{M}$ is given by $(x^\mu, q^A_{\mu_1\ldots\mu_r}, v^A_{\nu_1\ldots\nu_{r+1}})$, where

$$\begin{aligned} q &= \frac{1}{r!}q^A_{\mu_1\ldots\mu_r}(dx^{\mu_1}\wedge\ldots\wedge dx^{\mu_r})_x\otimes e_A\in\wedge^r T_x^*U\otimes V,\\ v &= \frac{1}{r!}v^A_{\nu_1\ldots\nu_{r+1}}dx^{\nu_1}_x\otimes(dx^{\nu_2}\wedge\ldots\wedge dx^{\nu_{r+1}})_x\otimes e_A\in\wedge^r T_x^*U\otimes T_x^*U\otimes V, \end{aligned}$$

with e_A, $1\le A\le m$, a choice of basis on V. A field $\phi\in\Gamma(\wedge^r\mathcal{M}\otimes(\mathcal{M}\times V))$, with $\wedge^r\mathcal{M}\otimes(\mathcal{M}\times V) := \coprod_{x\in\mathcal{M}}\wedge^r T_x^*\mathcal{M}\otimes V$, is sometimes called a V-valued r-form on $\mathcal{M}$. When $r=0$, $\Gamma(\wedge^0\mathcal{M}\otimes(\mathcal{M}\times V))\cong C^\infty(\mathcal{M};V)$, which is the space of smooth functions with values in V. We will shorten the notation by writing $\Omega^r(\mathcal{M};V)$ for the space of fields.

Note that the Euler–Lagrange generalize in this setting to:

$$\frac{\partial\mathcal{L}}{\partial q^A_{\nu_1\ldots\nu_r}}\circ(\phi,\nabla\phi) - \nabla_\nu\left(\frac{\partial\mathcal{L}}{\partial v^A_{\nu\nu_1\ldots\nu_r}}\circ(\phi,\nabla\phi)\right) = 0. \tag{3.9}$$

Exercise: Show this.

We consider *one-parameter group action* Ψ *on* $\Omega^r(\mathcal{M})$, which is defined as follows:

$$\begin{aligned} \Psi:\mathbb{R}\times\Omega^r(\mathcal{M};V)&\to\Omega^r(\mathcal{M};V),\\ \Psi(s,\cdot):=\Psi_s:\Omega^r(\mathcal{M};V)&\to\Omega^r(\mathcal{M};V)\quad(s\in\mathbb{R}),\\ \Psi_0&=\mathrm{id}_{\Omega^r(\mathcal{M};V)},\\ \Psi_{s+t}&=\Psi_s\circ\Psi_s\quad\text{for all } s,t\in\mathbb{R}. \end{aligned}$$

We will be interested in one-parameter group actions for which the following map is well-defined:

$$\begin{aligned} \frac{d}{ds}|_{s=0}\Psi_s&:\Omega^r(\mathcal{M};V)\to\Omega^r(\mathcal{M};V),\\ \frac{d}{ds}|_{s=0}\Psi_s(\phi)(x)&=\lim_{s\to0}\frac{(\Psi_s\circ\phi)(x)-\phi(x)}{s}. \end{aligned}$$

In the above expression, we take the limit with respect to any choice of norm on $\wedge^r T_x^*\mathcal{M}\otimes V$, as the norms on finite dimensional vector spaces are all equivalent.

If $\frac{d}{ds}\Big|_{s=s_0}\Psi_s(\phi)\in\Omega^r(\mathcal{M};V)$, we say the one-parameter group action on $\Omega^r(\mathcal{M})$ is *differentiable at* $s=0$.

Example 3.4 (External transformations)**.** *Let $\psi_s:\mathcal{M}\to\mathcal{M}$ be a 1-parameter group of diffeomorphisms (a global flow on $\mathcal{M}$). Then the pullbacks*

$$\psi_s^*:\Omega^r(\mathcal{M};V)\to\Omega^r(\mathcal{M};V)$$

also form a 1-parameter group, which is differentiable at $s=0$, with

$$\frac{d}{ds}\Big|_{s=0}\psi_s^*\phi = L_X\phi,$$

where $X\in\mathcal{T}(\mathcal{M})$, such that $X(f)=\frac{d}{ds}|_{s=0}f(\psi_s)$ for all $f\in C^\infty(\mathcal{M})$, i.e. $X_x=\dot\gamma_x(0)$, for a smooth curve γ_x on $\mathcal{M}$ with $\gamma(t)=\psi_t(x)$.

Group actions of the form $\Psi_s=\psi_s^*$ are sometimes called external transformations*.*

Example 3.5 (Internal transformations)**.** *Let $T : \mathbb{R} \times GL(V) \to GL(V)$ be a one-parameter group action, with $T_s = T(s, \cdot)$, such that $\frac{d}{ds}\Big|_{s=s_0} T_s : V \to V$ is a well-defined linear map. Let*

$$\Psi_s : \Omega^r(\mathcal{M}; V) \to \Omega^r(\mathcal{M}; V)$$
$$\Psi_s(\phi^A \otimes e_A) = \phi^A \otimes T_s(e_A).$$

Then Ψ_s define a one-parameter group action. Furthermore,

$$\frac{d}{ds}\Big|_{s=0} \Psi_s(\phi) = \phi^A \otimes \left(\frac{d}{ds}\Big|_{s=0} T_s\right)(e_A) \in \Omega^r(\mathcal{M}; V).$$

These type of 1-parameter groups of diffeomorphisms (which do not arise from diffeomorphisms in spacetime) are sometimes called internal transformations.

Definition 3.5. *Let $\Psi : \mathbb{R} \times \Omega^r(\mathcal{M}; V) \to \Omega^r(\mathcal{M}; V)$ be a one-parameter group action. We say Ψ is a* symmetry transformation of $\mathcal{S}$ *if for all $s \in \mathbb{R}$ and all $\phi \in \Omega^r(\mathcal{M}; V)$:*

$$\mathcal{S}(\Psi_s \circ \phi) = \mathcal{S}(\phi).$$

Suppose that Ψ is a symmetry transformation of $\mathcal{S}$ such that $\frac{d}{ds}|_{s=0}\Psi_s : \Omega^r(\mathcal{M}; V) \to \Omega^r(\mathcal{M}; V)$ is well-defined, and if $\mathcal{L}$ denotes the corresponding Lagrangian. Then for all $\phi \in \Omega^r(\mathcal{M}; V)$

$$\int_{\mathcal{M}} \left[\frac{d}{ds}\Big|_{s=0} \mathcal{L} \circ (\Psi_s(\phi), \nabla\Psi_s(\phi))\right] \epsilon = 0.$$

The above statement is *consistent* with the following: then there exists a $\mathbb{F} \in \mathcal{T}(\mathcal{M})$ with $\mathbb{F}|_{\partial M} = 0$ if $\partial M \neq \emptyset$ such that

$$\frac{d}{ds}\Big|_{s=0} \mathcal{L} \circ (\Psi_s(\phi), \nabla\Psi_s(\phi)) = \operatorname{div} \mathbb{F}. \tag{3.10}$$

Indeed, this follows by integrating both sides of (3.10) over $\mathcal{M}$ with respect to the natural volume form ϵ and applying the divergence theorem.

Motivated by (3.10), we will define an *infinitesimal symmetry* as an analogue of (3.10) for transformations of the form $\Psi_s(\phi) = \phi + s\frac{d}{ds}|_{s=0}\Psi_s(\phi)$. That is to say, we will ignore the terms of "order $o(s)$" (little o-notation) that would appear formally in an expansion of a general $\Psi_s(\phi)$ around $s = 0$, if we were to equip $\Omega^r(\mathcal{M})$ with a norm:

$$\Psi_s(\phi) = \phi + s\frac{d}{ds}|_{s=0}\Psi_s(\phi) + o(s).$$

Definition 3.6. *Let $\Psi : \mathbb{R} \times \Omega^r(\mathcal{M}; V) \to \Omega^r(\mathcal{M}; V)$ be a one-parameter group action. We say Ψ is an* infinitesimal symmetry tranformation of $\mathcal{S}$ *if there exists an $\mathbb{F} \in \mathcal{T}(\mathcal{M})$ such that*

$$\frac{d}{ds}\Big|_{s=0} \mathcal{L} \circ \left(\phi + s\frac{d}{ds}|_{s=0}\Psi_s(\phi), \nabla\phi + s\nabla\frac{d}{ds}|_{s=0}\Psi_s(\phi)\right) = \operatorname{div} \mathbb{F}.$$

Theorem 3.7 (Noether's theorem for fields)**.** *Let Ψ be an infinitesimal symmetry of $\mathcal{S}$ and define $\mathbb{J} \in \mathcal{T}(\mathcal{M})$ as follows: with respect to a coordinate chart $(U, \{x^\mu\})$, we can express $\mathbb{J} = \mathbb{J}^\mu \partial_{x^\mu}$, where*

$$\mathbb{J}^\nu = \frac{\partial \mathcal{L}}{\partial v^B_{\nu\nu_1\ldots\nu_r}} \circ (\phi, \nabla\phi) \left(\frac{d}{ds}|_{s=0}\Psi_s(\phi)\right)^B_{\nu_1\ldots\mu_r} - \mathbb{F}^\nu,$$

with ϕ a solution to the Euler–Lagrange equations on U. Then

$$\operatorname{div} \mathbb{J} = 0.$$

We refer to $\mathbb{J}$ as a conserved current.

Proof. Denote $h = \frac{d}{ds}\Big|_{s=0} \Psi_s(\phi)$ and consider the field $\phi + sh$. By using the infinitesimal symmetry property and applying the chain rule, we obtain in U

$$\begin{aligned}\operatorname{div} \mathbb{F} = \frac{d}{ds}\Big|_{s=0} \mathcal{L} \circ (\phi + sh, \nabla(\phi + sh)) &= \frac{\partial \mathcal{L}}{\partial q^B_{\nu_1 \dots \nu_r}}(\phi, \nabla\phi) h^B_{\nu_1 \dots \nu_r} + \frac{\partial \mathcal{L}}{\partial v^B_{\nu\nu_1 \dots \nu_r}}(\phi, \nabla\phi) \nabla_\nu h^B_{\nu_1 \dots \mu_r} \\ &= \left[\frac{\partial \mathcal{L}}{\partial q^B_{\nu_1 \dots \nu_r}}(\phi, \nabla\phi) - \nabla_\nu \left(\frac{\partial \mathcal{L}}{\partial v^B_{\nu\nu_1 \dots \nu_r}}(\phi, \nabla\phi) \right) \right] h^B_{\nu_1 \dots \mu_r} \\ &+ \nabla_\nu \left(\frac{\partial \mathcal{L}}{\partial v^B_{\nu\nu_1 \dots \nu_r}} \circ (\phi, \nabla\phi) h^B_{\nu_1 \dots \mu_r} \right).\end{aligned}$$

If ϕ is a solution to the Euler–Lagrange equations in U, then term inside the square brackets vanishes and we conclude that

$$\nabla_\nu \left(\frac{\partial \mathcal{L}}{\partial v^B_{\nu\nu_1 \dots \nu_r}} \circ (\phi, \nabla\phi) h^B_{\nu_1 \dots \mu_r} - \mathbb{F}^\nu \right) = 0. \qquad \square$$

Example 3.6. *Recall Example 3.1: let $\mathcal{M} = \mathbb{R}^{n+1}$ and $r = 0$. Then $\mathcal{N} \cong \mathbb{R}^{n+1} \times \mathbb{R} \times \mathbb{R}^{n+1}$. Let $\{x^\mu\}$ be Cartesian coordinates and m the Minkowski metric. Consider*

$$\mathcal{L} : \mathcal{N} \to \mathbb{R}, \quad \text{with}$$
$$\mathcal{L}(x, q, v) = \frac{1}{2} m_x^{-1}(v, v) + \frac{\mathfrak{m}^2}{2} q^2,$$

with $\mathfrak{m} \in \mathbb{R}$. Then $\mathcal{L}((\phi, \nabla\phi)(x)) = \frac{1}{2} m_x^{-1}(\nabla\phi(x), \nabla\phi(x)) + \frac{\mathfrak{m}^2}{2}\phi^2(x)$.

We consider the one-parameter group of diffeomorphisms $\psi : \mathbb{R} \times \mathbb{R}^{n+1} \to \mathbb{R}^{n+1}$ corresponding to spacetime translations in an arbitrary direction $b \in \mathbb{R}^{n+1}$. In Cartesian coordinates, this takes the form:

$$\psi_s(x^0, \dots, x^n) = (x^0 + sb^0, \dots, x^n + sb^n).$$

We will write $x + sb$ for $\psi_s(x)$ and interpret b also as a vector field on $\mathbb{R}^{n+1}$.

Then $\frac{d}{ds}|_{s=0}(\psi_s^* \phi) = L_b \phi$ and

$$\nabla \frac{d}{ds}|_{s=0}(\psi_s^* \phi) = \nabla L_b \phi = L_b \nabla \phi.^{12}$$

So for $h = \frac{d}{ds}|_{s=0}(\psi_s^* \phi)$:

$$\begin{aligned}\frac{d}{ds}|_{s=0} \mathcal{L} \circ (\phi + sh, \nabla\phi + s\nabla h) &= m^{-1}(\nabla\phi, \nabla h) + \mathfrak{m}^2 \phi h \\ &= m^{-1}(\nabla\phi, L_b \nabla\phi) + \mathfrak{m}^2 \phi L_b \phi \\ &= L_b(\mathcal{L} \circ (\phi, \nabla\phi)) - \frac{1}{2} L_b(m^{-1})(\nabla\phi, \nabla\phi).\end{aligned}$$

and, since $L_b(m^{-1}) = \frac{d}{ds}|_{s=0} \psi_s^* m^{-1} = 0$, and $\psi_s^* m^{-1} = m^{-1}$, i.e. ψ_s is an isometry of the Minkowski spacetime, we therefore have that

$$\frac{d}{ds}|_{s=0} \mathcal{L} \circ (\phi + sh, \nabla\phi + s\nabla h) = b^\mu \nabla_\mu (\mathcal{L} \circ (\phi, \nabla\phi)) = \nabla_\mu (b^\mu \mathcal{L} \circ (\phi, \nabla\phi)).$$

We therefore have that Ψ defined by $\Psi_s = \psi_s^*$ is an infinitesimal symmetry with $\mathbb{F}^\mu_0 = b^\mu \mathcal{L} \circ (\phi, \nabla\phi)$.

By Noether's theorem, the conserved current J takes the form with respect to Cartesian coordinates:

$$\mathbb{J}^\mu = \frac{\partial \mathcal{L}}{\partial v_\mu} \circ (\phi, \nabla\phi) b^\nu \partial_\nu \phi - \mathbb{F}^\mu = b^\nu \nabla^\mu \phi \nabla_\nu \phi - b^\mu \frac{1}{2} \left((m^{-1})^{\alpha\beta} \partial_\alpha \phi \partial_\beta \phi + \mathfrak{m}^2 \phi^2 \right),$$

with ϕ a solution to the E–L equations.

[12] Exercise: Show that $[L_X, \nabla] = [L_X, d] = 0$ when acting on functions.

Since b was arbitrary and constant, we can write $\mathbb{J}_\mu = b^\nu \mathbb{T}_{\mu\nu}$, with

$$\mathbb{T}_{\mu\nu} = \partial_\mu\phi\partial_\nu\phi - \frac{1}{2}m_{\mu\nu}\left((m^{-1})^{\alpha\beta}\partial_\alpha\phi\partial_\beta\phi + \frac{\mathfrak{m}^2}{2}\phi^2\right).$$

Then $\nabla^\mu\mathbb{T}_{\mu\nu} = 0$. The tensor field

$$\mathbb{T} = \mathbb{T}_{\mu\nu}dx^\mu \otimes dx^\nu$$

is called the stress-energy tensor *or* energy-momentum tensor*. The key property of the stress-energy tensor is that it is* divergence-free *(i.e. $\nabla^\mu\mathbb{T}_{\mu\nu} = 0$).*

We refer to

$$E(t) = \int_{\mathbb{R}^n} \mathbb{T}^{00}|_{x^0=t}\, d\mathbf{x}$$

as the energy of ϕ at time t and

$$P^i(t) = \int_{\mathbb{R}^n} \mathbb{T}^{0i}|_{x^0=t}\, d\mathbf{x}$$

as the i-th component of the linear momentum of ϕ at time t.

Example 3.7. *We consider the 1-parameter group of diffeomorphisms $\psi_s : \mathbb{R}^{n+1} \to \mathbb{R}^{n+1}$ corresponding to Lorentz transformations. In Cartesian coordinates, these take the form:*

$$\psi_s^\mu(x) = \Lambda_\nu^\mu(s)x^\nu,$$

where $\Lambda_\nu^\mu(s)$ are the components of a 1-parameter group of proper, ortochronous Lorentz transformations $\Lambda(s) \in SO^+(n;1)$ It will be useful to characterize $O(n;1)$ as follows $O(n;1) = \{\Lambda \in GL(n+1;\mathbb{R}) \,|\, \Lambda^T\eta\Lambda = \eta\}$, with η the diagonal matrix with entries $-1, +1, \ldots, +1$. Then $\Lambda \in SO^+(n;1)$ if additionally $\det\Lambda = 1$ and $\Lambda_{00} > 0$.

We will write $\Lambda(s)x$ for $\psi_s(x)$. Note that

$$\frac{d}{ds}\Big|_{s=0}\psi_s^\mu(x) = \frac{d}{ds}|_{s=0}(\Lambda_\nu^\mu(s)x^\nu) = A_\nu^\mu x^\nu,$$

with $A \in \mathfrak{so}(n;1) = \{A \in \mathrm{Mat}(n+1;\mathbb{R}) \,|\, \eta A^T\eta = -A\}$,[13] *where $\mathfrak{so}(1,n)$ is the Lie algebra corresponding to $SO(n;1)$. In fact, for any $A \in \mathfrak{so}(1,n)$, the matrix exponential $\Lambda(s) = \exp(sA)$ defines a 1-parameter group of Lorentz transformations such that $\frac{d}{ds}|_{s=0}\Lambda(s) = A$.*

Then, for $X = A_\nu^\mu x^\nu\partial_{x^\mu}$,

$$\frac{d}{ds}|_{s=0}\psi_s^*\phi = \frac{d}{ds}|_{s=0}\phi\circ\psi_s = \frac{d}{ds}|_{s=0}\psi_s^\mu\partial_\mu\phi = L_X\phi = X(\phi)$$

and

$$\nabla\frac{d}{ds}|_{s=0}(\psi_s^*\phi) = \nabla L_X\phi = L_X\nabla\phi,$$

so just like in the previous example, we obtain for $h = \frac{d}{ds}|_{s=0}(\psi_s^*\phi)$:

$$\frac{d}{ds}|_{s=0}\mathcal{L}\circ(\phi + sh, \nabla\phi + s\nabla h) = L_X(\mathcal{L}\circ(\phi,\nabla\phi)) - \frac{1}{2}L_X(m^{-1})(\nabla\phi,\nabla\phi).$$

In this case, we use the expression for the pullback in coordinates:

$$(\psi_s^*m)_{\mu\nu} = \frac{\partial\psi_s^\alpha}{\partial x^\mu}\frac{\partial\psi_s^\beta}{\partial x^\nu}m_{\alpha\beta} = \Lambda(s)_\mu^\alpha m_{\alpha\beta}\Lambda(s)_\nu^\beta = (\Lambda^T\eta\Lambda)_{\mu\nu} = m_{\mu\nu},$$

so $L_Xm = 0$ and we conclude that

$$\begin{aligned}\frac{d}{ds}|_{s=0}\mathcal{L}\circ(\phi + sh, \nabla\phi + s\nabla h) &= L_X(\mathcal{L}\circ(\phi,\nabla\phi))\\ &= A_\nu^\mu x^\nu\partial_\mu((\mathcal{L}\circ(\phi,\nabla\phi)))\\ &= x^\nu\partial_\mu(A_\nu^\mu(\mathcal{L}\circ(\phi,\nabla\phi))),\end{aligned}$$

[13] By definition of Lorentz transformations $\frac{d}{ds}|_{s=0}(\Lambda^T(s)\eta\Lambda(s)) = 0$. Since taking the transpose of a matrix is a linear operation, we have that for $A = \frac{d}{ds}|_{s=0}\Lambda(s))$, $A^T\eta + \eta A = 0$. Equivalently, since $\eta = \eta^{-1}$, $\eta A^T\eta = -A$.

Using that $\operatorname{tr}(A) = -\operatorname{tr}(\eta A \eta) = -\operatorname{tr} A$*, we have that* $\operatorname{tr} A = 0$*, so we can further rewrite:*

$$x^\nu \partial_\mu (A^\mu_\nu (\mathcal{L} \circ (\phi, \nabla\phi)))(x) = \partial_\mu (A^\mu_\nu x^\nu (\mathcal{L} \circ (\phi, \nabla\phi))).$$

Hence,

$$\mathbb{F}^\mu(x) = A^\mu_\nu x^\nu \mathcal{L}(\phi(x), \nabla\phi(x))$$

and in analogy with the previous example,

$$\begin{aligned}\mathbb{J}^\mu(x) &= \frac{\partial \mathcal{L}}{\partial v_\mu}(\phi(x), \nabla\phi(x)) A^\alpha_\nu x^\nu \partial_\alpha \phi(x) - \mathbb{F}^\mu(x) \\ &= A^\nu_\beta x^\beta \mathbb{T}^\mu{}_\nu.\end{aligned}$$

Since the dimension of $\mathfrak{so}(n;1)$ *is* $\frac{1}{2}(n+1)n$*, there are* $\frac{1}{2}n(n+1)$ *linearly independent conserved currents associated to* $SO(n;1)$*. For example, we can label:*

$$({}^{\alpha\beta}\mathbb{J})^\mu(x) = x^\alpha \mathbb{T}^{\mu\beta}(x) - x^\beta \mathbb{T}^{\mu\alpha}(x),$$

which are antisymmetric in α, β *and therefore result in* $\frac{1}{2}(n+1)n$ *linearly independent currents.*

The following $\frac{1}{2}n(n-1)$ *quantities can be associated to the rotation subgroup* $SO(n) \subseteq SO(n;1)$*:*

$$Q^{ij}(t) = \int_{\mathbb{R}^3} ({}^{ij}\mathbb{J})^0|_{x^0=t}\, d\mathbf{x} = \int_{\mathbb{R}^3} (x^i \mathbb{T}^{0j} - x^j \mathbb{T}^{0i})|_{x^0=t}\, d\mathbf{x}$$

and can be interpreted as the angular momentum of ϕ *at time* t*. The following* n *quantities are associated to Lorentz boosts:*

$$Q^{0i}(t) = \int_{\mathbb{R}^3} ({}^{0i}J)^0\, d\mathbf{x} = \int_{\mathbb{R}^3} (x^0 T^{0i} - x^i T^{00})(\phi(x), \nabla\phi(x))\, d\mathbf{x}.$$

Proposition 3.8. *Suppose* $\phi(t, \mathbf{x})$ *and* $\nabla\phi(t, \mathbf{x})$ *go to zero as* $|\mathbf{x}| \to \infty$*. Then* $E(t)$*,* $P_i(t)$*,* $Q^{ij}(t)$ *and* $Q^{0i}(t)$ *are conserved in time.*

Proof. Exercise. □

Example 3.8. *Let* $\mathcal{M} = \mathbb{R}^{n+1}$*,* $r = 0$ *and* $V = \mathbb{R}^2$*. We can identify* $\mathbb{R}^2$ *with* $\mathbb{C}$ *by letting* $q^1 = \Re(q)$ *and* $q^2 = \Im(q)$*, for* $q \in \mathbb{R}^2$*. Consider the Lagrangian:*

$$\begin{aligned}\mathcal{L} &: \mathcal{N} \to \mathbb{R}, \\ \mathcal{L}(x, q, v) &= \frac{1}{2} m_x^{-1}(v^1, v^1) + \frac{1}{2} m_x^{-1}(v^2, v^2) + \frac{\mathfrak{m}^2}{2}|q|^2.\end{aligned}$$

Let $\phi \in C^\infty(\mathbb{R}^{n+1}; \mathbb{C})$ *be a complex-valued field. Then, we consider the following one-parameter group action:* $\Psi_s : C^\infty(\mathbb{R}^{n+1}; \mathbb{C}) \to C^\infty(\mathbb{R}^{n+1}; \mathbb{C})$*, with*

$$\Psi_s(\phi)(x) = e^{is}\phi(x).$$

Then

$$\begin{aligned}\frac{d}{ds}\Big|_{s=0} \Psi_s(\phi) &= i\phi, \\ \nabla \frac{d}{ds}\Big|_{s=0} \Psi_s(\phi) &= i\nabla\phi,\end{aligned}$$

so for $h = \frac{d}{ds}\Big|_{s=0} \Psi_s(\phi) = i\phi = -\phi^2 + i\phi^1$*,*

$$\frac{d}{ds}|_{s=0} \mathcal{L} \circ (\phi + sh, \nabla\phi + s\nabla h) = m^{-1}(\nabla\phi^1, \nabla h^1) + m^{-1}(\nabla\phi^2, \nabla h^2) + \mathfrak{m}^2 \Re(\phi\overline{h}) = 0,$$

so $\mathbb{F} = 0$*.*

The corresponding Noether current is given by:

$$\mathbb{J}^\mu = \frac{\partial \mathcal{L}}{\partial v^B_\mu} \circ (\phi, \nabla\phi) \left(\frac{d}{ds}|_{s=0} \Psi_s(\phi) \right)^B = \Re(\nabla^\mu\phi)(x)\Re(i\phi)(x) + \Im(\nabla^\mu\phi)(x)\Im(i\phi) = \Im(\overline{\phi}\nabla^\mu\phi).$$

3.4 The Einstein–Hilbert action

We will now show that we can also derive the *Einstein equations of general relativity*, by extremizing an appropriate action. We start by considering the action corresponding to a field $\phi \in \Omega^r(\mathcal{M})$ with $(\mathcal{M}, g)$ an orientable $n+1$-dimensional Lorentzian manifold. Rather than keeping g fixed, we will be considering one-parameter families of Lorentzian metrics on a fixed manifold $\mathcal{M}$.[14]

$$\mathcal{S}_{\text{matter}}(\phi, g) = \int_{\mathcal{M}} \mathcal{L}_{\text{matter}} \circ (\phi, \nabla^g \phi, g)\, \epsilon[g],$$

with $\epsilon[g]$ the natural volume form associated to g, ∇^g the covariant derivative associated to the Levi–Civita connection corresponding to g and

$$\begin{aligned} &\mathcal{L}_{\text{matter}} : \mathcal{N} \to \mathbb{R}, \\ &\mathcal{N} := \coprod_{x \in \mathcal{M}} (\wedge^r T_x^* \mathcal{M}) \times (T_x^* \mathcal{M} \otimes \wedge_x^r T^* \mathcal{M}) \times \text{Lor}_x, \end{aligned}$$

with Lor_x the set of symmetric, non-degenerate elements of $T_x^* M \otimes T_x^* M$ with signature $(- + \ldots +)$.

We will assume that $\mathcal{L}_{\text{matter}}(\cdot, \nabla^{g_1}\phi, \cdot) = \mathcal{L}_{\text{matter}}(\cdot, \nabla^{g_2}\phi, \cdot)$ for any two Lorentzian metrics g_1 and g_2 and $\phi \in \Omega^r(\mathcal{M})$! All the Lagrangians we have encountered so far satisfy this property.

For example, we could consider a Klein–Gordon Lagrangian, which satisfies:

$$\mathcal{L}_{\text{matter}}(x, q, v, k) = \frac{1}{2} k^{-1}(v, v) + \frac{\mathfrak{m}^2}{2} q^2,$$

with $k^{-1} \in T_x\mathcal{M} \otimes T_x\mathcal{M}$ the unique tensor associated to $k \in \text{Lor}_x$ via musical isomorphisms induced by k. In this case $\nabla^{g_1}\phi = d\phi = \nabla^{g_2}\phi$ for any two Lorentzian metrics g_1, g_2.

The *equations of motion* of ϕ are the Euler–Lagrange equations corresponding to $\mathcal{S}_{\text{matter}}$. Since they depend on on the metric g, they can be thought of describing how the behaviour of the field on $(\mathcal{M}, g)$ is affected by the curvature of $(\mathcal{M}, g)$ ("spacetime tells matter how to move"). In §3.2, we showed that they can be derived by considering $\frac{d}{ds}|_{s=0}\mathcal{S}_{\text{matter}}(\phi + sh, g)$, with h and its derivatives vanishing at the boundary $\partial\mathcal{M}$.

The Einstein equations describe instead how the metric g is affected by the presence of the field ϕ ("matter tells spacetime how to curve"). We will derive them by defining the following *total action*:

$$\mathcal{S}(\phi, g) = -\frac{1}{16\pi} \int_{\mathcal{M}} R[g]\, \epsilon[g] + \mathcal{S}_{\text{matter}}(\phi, g),$$

where $R[g]$ is the Ricci scalar corresponding to the metric g and considering $\frac{d}{ds}|_{s=0}\mathcal{S}(\phi, g+sh)$ with $h|_{\partial\mathcal{M}} \equiv 0$. The part of the action

$$\mathcal{S}_{\text{EH}}(g) := \frac{1}{16\pi} \int_{\mathcal{M}} R[g]\, \epsilon[g]$$

is called the *Einstein–Hilbert action.*

Remark 3.1. *The Ricci scalar R is a smooth function on $(\mathcal{M}, g)$ that is invariant under isometries by Proposition A.9 in the appendix. It is not the unique function on $\mathcal{M}$ with that property. We could have, for example, also considered contractions of the Riemann tensor $R_{\mu\nu\alpha\beta}R^{\mu\nu\alpha\beta}$ or the Ricci tensor $R_{\mu\nu}R^{\mu\nu}$ or functions thereof.*

We will restrict to a compact subset $\mathcal{K} \subset \mathcal{M}$. Let g be a Lorentzian metric and consider the one-parameter family of tensor fields $g^s = g + sh \in \mathcal{T}^{(0,2)}(\mathcal{K})$, with $h \in \mathcal{T}^{(0,2)}(\mathcal{K})$ symmetric and $s \in I \subset \mathbb{R}$ suitably small (depending on g) such that g^s is a Lorentzian metric. If K has a boundary, then we will also assume that

[14] It is at this point good to point out that not every manifold admits a Lorentzian metric $\mathcal{M}$, let alone a one-parameter family of Lorentzian metrics. If $\mathcal{M}$ is covered by a single coordinate chart $\{x^\mu\}$, however, we can express $g = g_{\alpha\beta}dx^\alpha \otimes dx^\beta$ and there is a bijection between the set of Lorentzian metrics and the set of smooth, symmetric, non-degenerate, matrix-valued functions, which can trivially be constructed.

h is supported in a compact subset of the interior of $\mathcal{K}$ so that $h_{\mu\nu}$ and $\partial_\rho h_{\mu\nu}$ vanish at the boundary $\partial\mathcal{K}$ with respect to an arbitrary coordinate chart.

Since we have that, schematically,

$$\begin{aligned}\text{Riem} &= \partial\Gamma + \Gamma\Gamma,\\ \Gamma &= g^{-1}\partial g\end{aligned}$$

in the domain of a coordinate chart, we can see that $R[g]$ does not just depend on g and its partial derivatives, but it also depends on **second-order derivatives of** g. In view of our derivation of the Euler–Lagrange equations for general Lagrangians (with covariant derivatives replaced by partial derivatives), we might expect to obtain *third-order* equations of motion for the components of g (as the Euler–Lagrange equations corresponding to Lagrangians depending on the field and its first-order derivatives resulted in second-order equations). We will see however, that the equations of motion are in fact second order.

Lemma 3.9. *With respect to an arbitrary coordinate chart (U, x^μ), we can express*

$$\frac{d}{ds}\Big|_{s=0}\epsilon[g^s] = \frac{1}{2}(g^{-1})^{\mu\nu}h_{\mu\nu}\,\epsilon[g].$$

Proof. We have that with respect an arbitrary coordinate chart (U, x^μ):

$$\epsilon[g^s] = \sqrt{-\det g^s}dx^0 \wedge \ldots \wedge dx^n.$$

From the chain rule, it follows that

$$\frac{d}{ds}\Big|_{s=0}\sqrt{-\det g^s} = -\frac{1}{2}(-\det g)^{-\frac{1}{2}}\frac{d}{ds}\Big|_{s=0}\det g^s.$$

We use the following fact from linear algebra. For any symmetric $(n+1)\times(n+1)$ matrix Y, we have that:[15]

$$\det e^Y = e^{\operatorname{tr} Y}.$$

This follows immediately by using that a symmetric matrix Y can be written as $Y = B^{-1}DB$, where D is diagonal, and $e^Y = e^{B^{-1}DB} = B^{-1}e^D B$. In fact the identity holds also for general matrices, but we will not need that fact.

Let A, X be a symmetric matrices and consider $A_s := A + sX = A(\mathbf{1} + sA^{-1}X)$. We obtain

$$A_s = Ae^{sA^{-1}X}(\mathbf{1} + B_s),$$

where $B_0 = 0$ and $\frac{d}{ds}|_{s=0}B_s = 0$.

Hence,

$$\det A_s = \det A \det(e^{sA^{-1}X})\det(I + B_s).$$

We therefore have that

$$\frac{d}{ds}|_{s=0}\det A_s = \det A\frac{d}{ds}|_{s=0}\det(e^{sA^{-1}X}) = \frac{d}{ds}|_{s=0}e^{s\operatorname{tr}(A^{-1}X)} = \operatorname{tr}(A^{-1}X)\det A.$$

Hence, $\frac{d}{ds}|_{s=0}\det g_s = (g^{-1})^{\mu\nu}h_{\mu\nu}\det g$ and we conclude that

$$\frac{d}{ds}\Big|_{s=0}\sqrt{-\det g^s} = \frac{1}{2}\sqrt{-\det g}(g^{-1})^{\mu\nu}h_{\mu\nu}.$$ □

Lemma 3.10. (i) *Denote with $\Gamma^\rho_{\mu\nu}[g^s]$ the Christoffel symbols with respect to g^s. Then with respect to an arbitrary coordinate chart*

$$\frac{d}{ds}\Big|_{s=0}\Gamma^\rho_{\mu\nu}[g^s] = \frac{1}{2}(g^{-1})^{\rho\sigma}(\nabla_\nu h_{\mu\sigma} + \nabla_\mu h_{\nu\sigma} - \nabla_\sigma h_{\mu\nu}),$$

where ∇ denotes the Levi–Civita covariant derivative with respect to g.

[15] The matrix exponent e^A of a general matrix A is given by $e^A = \sum_{n=0}^\infty \frac{A^n}{n!}$.

(ii) *For $R_{\mu\nu}[g^s]$ denoting the components of the Ricci tensors corresponding to the metrics g^s, we can express with respect to an arbitrary coordinate chart*

$$\frac{d}{ds}\Big|_{s=0} R[g^s] = -R_{\mu\nu}[g]h^{\mu\nu} + \nabla_\rho J^\rho,$$

with

$$J^\rho = \nabla^\mu h^\rho{}_\mu - \nabla^\rho h^\mu{}_\mu.$$

Proof. Recall that with respect to normal coordinates around a point $p \in \mathcal{M}$ corresponding to g: $g_{\mu\nu}(p) = m_{\mu\nu}$, $\Gamma^\rho_{\mu\nu} = 0$ and $\partial_\rho g_{\mu\nu}(p) = 0$. Hence,

$$\begin{aligned}\Gamma^\rho_{\mu\nu}[g^s](p) &= \frac{s}{2}(g^{-1})^{\rho\sigma}(p)(\partial_\nu h_{\mu\sigma} + \partial_\mu h_{\nu\sigma} - \partial_\sigma h_{\mu\nu})(p) + o(s),\\ &= \frac{s}{2}(g^{-1})^{\rho\sigma}(p)(\nabla_\nu h_{\mu\sigma} + \nabla_\mu h_{\nu\sigma} - \nabla_\sigma h_{\mu\nu})(p) + o(s),\end{aligned}$$

with $o(s)$ denoting terms that vanish in the limit $s \to 0$ and ∇ the covariant derivative with respect to g. We obtain

$$\frac{d}{ds}\Big|_{s=0} \Gamma^\rho_{\mu\nu}[g^s](p) = \frac{1}{2}(g^{-1})^{\rho\sigma}(\nabla_\nu h_{\mu\sigma} + \nabla_\mu h_{\nu\sigma} - \nabla_\sigma h_{\mu\nu})(p).$$

While the above expression was derived with respect to normal coordinates around p, it remains valid under a change of coordinates. Hence, we can define a tensor field $C \in \mathcal{T}^{(1,2)}(\mathcal{M})$ globally, with $C^\rho{}_{\mu\nu}$ equal to the right-hand side above in *any* coordinate chart. We conclude (i).

To obtain (ii), we turn again to normal coordinates around $p \in \mathcal{M}$ with respect to the metric g, in which the components of the Riemann tensor with respect to g^s, $R^\sigma{}_{\mu\rho\nu}[g^s]$, satisfy

$$R^\sigma{}_{\mu\rho\nu}[g^s](p) = \partial_\rho \Gamma^\sigma_{\nu\mu}[g^s](p) - \partial_\nu \Gamma^\sigma_{\rho\mu}[g^s](p).$$

and

$$R_{\mu\nu}[g^s](p) = \partial_\rho \Gamma^\rho_{\nu\mu}[g^s](p) - \partial_\nu \Gamma^\rho_{\rho\mu}[g^s](p).$$

Hence,

$$R[g^s](p) = ((g^s)^{-1})^{\mu\nu}(p) R_{\mu\nu}[g^s](p).$$

We therefore have that

$$\begin{aligned}\frac{d}{ds}\Big|_{s=0} R[g^s](p) &= R_{\mu\nu}[g](p)\frac{d}{ds}\Big|_{s=0}((g^s)^{-1})^{\mu\nu}(p) + (g^{-1})^{\mu\nu}\partial_\rho \frac{d}{ds}\Big|_{s=0}\Gamma^\rho_{\nu\mu}[g^s](p) - (g^{-1})^{\mu\nu}\partial_\nu \frac{d}{ds}\Big|_{s=0}\Gamma^\rho_{\rho\mu}[g^s](p)\\ &= R_{\mu\nu}[g](p)\frac{d}{ds}\Big|_{s=0}((g^s)^{-1})^{\mu\nu}(p) + \frac{1}{2}\nabla^\rho(\nabla^\mu h_{\mu\rho} + \nabla^\mu h_{\mu\rho} - \nabla_\rho h^\mu_\mu)(p)\\ &\quad - \frac{1}{2}\nabla^\mu(\nabla_\mu h^\rho_\rho + \nabla^\rho h_{\mu\rho} - \nabla^\rho h_{\rho\mu})(p)\\ &= R_{\mu\nu}[g](p)\frac{d}{ds}\Big|_{s=0}((g^s)^{-1})^{\mu\nu}(p) + \nabla^\rho(\nabla^\mu h_{\mu\rho} - \nabla_\rho h^\mu_\mu).\end{aligned}$$

Since $((g^s)^{-1})^{\mu\nu} g^s_{\nu\alpha} = \delta^\mu_\alpha$, we have that

$$g_{\nu\alpha}\frac{d}{ds}\Big|_{s=0}((g^s)^{-1})^{\mu\nu} = -(g^{-1})^{\mu\nu}\frac{d}{ds}\Big|_{s=0} g^s_{\nu\alpha} = -(g^{-1})^{\mu\nu}h_{\nu\alpha}$$

From this it follows that

$$\frac{d}{ds}\Big|_{s=0}((g^s)^{-1})^{\mu\nu} = -(g^{-1})^{\mu\alpha}(g^{-1})^{\nu\beta}h_{\alpha\beta} = -h^{\mu\nu}. \tag{3.11}$$

We conclude that

$$\frac{d}{ds}|_{s=0} R[g^s](p) = -R_{\mu\nu}[g]h^{\mu\nu} + \nabla_\rho J^\rho,$$

with

$$J^\rho = \nabla^\mu h^\rho_\mu - \nabla^\rho h^\mu_\mu.$$ □

Note that the term $\nabla_\rho J^\rho$ involves second-order derivatives of h, because it is the divergence of a vector field, there will be no need to integrate it by parts, since it will vanish after integration.

Proposition 3.11. *Assume that* $\mathcal{L}_{\text{matter}}(x, q, \nabla^{g_1}\phi(x), k) = \mathcal{L}_{\text{matter}}(x, q, \nabla^{g_2}\phi(x), k)$ *for all Lorentzian metrics* g_1, g_2, $\phi \in \Omega^r(\mathcal{M})$, $x \in \mathcal{M}$, $q \in \wedge^r(T_x\mathcal{M})$ *and* $k \in \text{Lor}_x$.

A pair $(\phi, g) \in \Omega^r(\mathcal{K}) \times \mathcal{T}^{(0,2)}(\mathcal{K})$, *with* g *a Lorentzian metric, is an extremum of* $\mathcal{S}(g, \phi)$ *restricted to a compact subset* $\mathcal{K} \subseteq \mathcal{M}$ *implies that in the interior of* $\mathcal{K}$*:*

$$G_{\mu\nu}[g] = 8\pi \mathbb{T}_{\mu\nu}[\phi, g], \tag{3.12}$$

$$\nabla_\mu \left(\frac{\partial \mathcal{L}_{\text{matter}}}{\partial v_{\mu\mu_1\dots\mu_r}} \circ (\phi, \nabla^g\phi, g) \right) - \frac{\partial \mathcal{L}_{\text{matter}}}{\partial q_{\mu_1\dots\mu_r}} \circ (\phi, \nabla^g\phi, g) = 0. \tag{3.13}$$

with

$$\mathbb{T}_{\mu\nu}[\phi, g] := 2 \left(\frac{\partial \mathcal{L}_{\text{matter}}}{\partial (k^{-1})^{\mu\nu}} \circ (\phi, \nabla^g\phi, g) - \frac{1}{2} g_{\mu\nu} \mathcal{L}_{\text{matter}} \circ (\phi, \nabla^g\phi, g) \right). \tag{3.14}$$

The equations (3.12) *are called* the Einstein equations of general relativity. *By the contracted Bianchi identity (Corollary A.11), we have that*

$$\nabla^\mu \mathbb{T}_{\mu\nu}[\phi, g] = 0.$$

We will refer to the corresponding tensor field $\mathbb{T}[\phi, g]$ *as the* Hilbert energy-momentum tensor *to contrast it with the energy-momentum tensor obtained from Noether's Theorem, which we will call the* Noether energy momentum-tensor.

Proof. By Lemma 3.9 and (ii) of Lemma 3.10, we have that

$$-\frac{d}{ds}\Big|_{s=0} \mathcal{S}_{\text{EH}}(g^s) = \frac{1}{16\pi} \int_{\mathcal{K}} (R_{\mu\nu}[g] - \frac{1}{2} g_{\mu\nu}) h^{\mu\nu} \, \epsilon[g] = \frac{1}{16\pi} \int_{\mathcal{K}} G_{\mu\nu}[g] h^{\mu\nu} \, \epsilon[g],$$

where we used the divergence theorem together with $J|_{\partial\mathcal{K}} = 0$ to conclude that the integral of $\nabla_\rho J^\rho$ vanishes.

We will now investigate $\mathcal{S}_{\text{matter}}$. By the chain rule, we have that

$$\frac{d}{ds}\Big|_{s=0} (\mathcal{L}_{\text{matter}} \circ (\phi, \nabla^{g^s}\phi, g^s) \epsilon[g^s]) = \frac{d}{ds}\Big|_{s=0} \mathcal{L}_{\text{matter}} \circ (\phi, \nabla^g\phi, g^s) \, \epsilon[g] + \mathcal{L}_{\text{matter}} \circ (\phi, \nabla^g\phi, g^s) \frac{d}{ds}\Big|_{s=0} \epsilon[g^s].$$

By applying (3.11), we therefore have that

$$\frac{d}{ds}\Big|_{s=0} \mathcal{L}_{\text{matter}} \circ (\phi, \nabla^g\phi, g^s) = -\frac{\partial \mathcal{L}_{\text{matter}}}{\partial (k^{-1})^{\mu\nu}} \circ (\phi, \nabla^g\phi, g) h^{\mu\nu},$$

where $h^{\mu\nu}$ are the components of the (2,0)-tensor field dual to h, defined via the musical isomorphisms with respect to g.

Together with Lemma 3.9, it follows therefore that

$$\frac{d}{ds}\Big|_{s=0} (\mathcal{L}_{\text{matter}} \circ (\phi, \nabla^g\phi, g^s) \epsilon[g^s]) = -\left(\frac{\partial \mathcal{L}_{\text{matter}}}{\partial (k^{-1})^{\mu\nu}} (\phi, \nabla^g\phi, g) - \frac{1}{2} g_{\mu\nu} \mathcal{L} \circ (\phi, \nabla^g\phi, g) \right) h^{\mu\nu} \, \epsilon[g].$$

Hence, $\frac{d}{ds}\Big|_{s=0} (\mathcal{L}_{\text{matter}} \circ (\phi, \nabla^g\phi, g^s) \epsilon[g^s]) = -\frac{1}{2} \mathbb{T}_{\mu\nu}[\phi, g] h^{\mu\nu}$, with

$$\mathbb{T}_{\mu\nu}[\phi, g] = 2 \left(\frac{\partial \mathcal{L}_{\text{matter}}}{\partial (k^{-1})^{\mu\nu}} \circ (\phi, \nabla^g\phi, g) - \frac{1}{2} g_{\mu\nu} \mathcal{L}_{\text{matter}} \circ (\phi, \nabla^g\phi, g) \right).$$

We then conclude that:

$$\frac{d}{ds}\Big|_{s=0} \mathcal{S}(\phi, g^s) = \frac{1}{16\pi} \int_{\mathcal{K}} (-8\pi \mathbb{T}_{\mu\nu}[\phi, g] + G_{\mu\nu}[g]) h^{\mu\nu} \, \epsilon[g].$$

Since h was arbitrary, we can apply Lemma 2.13 to the components $h^{\mu\nu}$ to conclude that (3.12) holds in the interior of $\mathcal{K}$.

We conclude (3.13) by instead considering $\frac{d}{ds}|_{s=0} \mathcal{S}_{\text{matter}}(\phi + s\psi, g)$, with $\psi \in \Omega^r(\mathcal{K})$, such that $\psi|_{\partial\mathcal{K}} \equiv 0$, which results in the Euler–Lagrange equations, as discussed in the previous chapters.

From the contracted Bianchi identity Corollary A.11 together with (3.12), it follows immediately that $\nabla^\mu \mathbb{T}_{\mu\nu}[\phi, g] = 0$. □

Remark 3.2. *The Hilbert energy-momentum tensor $\mathbb{T}$ is automatically symmetric, since the tensor G is symmetric. This $\mathbb{T}$ does not need to coincide with the Noether energy momentum tensor. As we have seen in Problem Sheet 8, the canonical energy-momentum tensor need not be symmetric. One can show that:*

$$\mathbb{T}^{\text{Hilbert}}_{\mu\nu} = \mathbb{T}^{\text{Noether}}_{\mu\nu} + \nabla_\lambda \mathbb{B}^\lambda{}_{\mu\nu},$$

for an appropriate choice of (1,2) tensor $\mathbb{B}$.[16]

The definition (3.14) therefore provides a convenient way of constructing symmetric energy-momentum tensors, even when one is only interested in the Euler–Lagrange equations with a fixed g. It moreover singles out a unique of energy-momentum tensor that is relevant when studying the interactions of the field theory with gravity.

Remark 3.3. *One can also study the gravitational properties of matter with equations of motions that do not arise from an action principle, by considering (3.12) with a given symmetric (0,2) tensor field $\mathbb{T}$ such that $\nabla_\mu \mathbb{T}^{\mu\nu} = 0$. For example, when studying the gravitational properties of fluids (Einstein–Euler equations).*

By redefining $\mathcal{S}_{\text{EH}}(g) := \frac{1}{16\pi}\int_{\mathcal{M}}(R[g] - 2\Lambda)\,\epsilon[g]$ with $\Lambda \in \mathbb{R}$ a constant, we obtain instead the equations:

$$G_{\mu\nu}[g] + \Lambda g_{\mu\nu} = 8\pi \mathbb{T}_{\mu\nu}[\phi, g]. \tag{3.15}$$

Exercise: Show this.

The constant Λ is called a *cosmological constant* and it plays an important role when gravitational properties at a cosmological scale, where $\Lambda > 0$ (and very small) must be included to account for experimental observations at cosmological scales. By putting the $\Lambda g_{\mu\nu}$ on the right-hand side of the equation with $8\pi\mathbb{T}_{\mu\nu}$, it can be interpreted as part of the energy-momentum tensor. It is therefore often referred to as *dark energy*.

In four spacetime dimensions, the Einstein equations with cosmological constant are the most general equations with a symmetric, divergence-free (0,2)-tensor on the left-hand side:

Theorem 3.12 (Lovelock's Theorem)**.** *Let $(\mathcal{M}, g)$ be a four-dimensional Lorentzian manifold. Let $H \in \mathcal{T}^{(0,2)}(\mathcal{M})$ be symmetric and divergence free ($\nabla^\mu H_{\mu\nu} = 0$), such for any $p \in \mathcal{M}$ and with respect to any coordinate chart with domain containing p, $H_{\mu\nu}(p)$ can be expressed as a function of $g_{\mu\nu}(p)$, $\partial_\rho g_{\mu\nu}(p)$ and $\partial_\sigma\partial_\rho g_{\mu\nu}(p)$. Then, there exist $\alpha, \beta \in \mathbb{R}$, such that*

$$H_{\mu\nu} = \alpha G_{\mu\nu} + \beta g_{\mu\nu}.$$

4 Gauge theories

4.1 Gauge transformations in electromagnetism

We consider the electromagnetic Lagrangian from Example 3.2, which corresponds to the Maxwell equations of electromagnetism in vacuum, but we replace $(\mathbb{R}^{n+1}, m)$ by a general Lorentzian manifold $(\mathcal{M}, g)$:

$$\begin{aligned}
\mathcal{L} : \mathcal{N} &\to \mathbb{R}, \quad \text{with} \\
\mathcal{N} &= \coprod_{x\in\mathcal{M}} \wedge^1 T^*_x\mathcal{M} \times (T^*_x\mathcal{M} \otimes \wedge^1 T^*_x\mathcal{M}), \\
\mathcal{L}(x, q, v) &= -\frac{1}{4}(g^{-1})^{\alpha\mu}_x (g^{-1})^{\beta\nu}_x (v_{\mu\nu} - v_{\nu\mu})(v_{\alpha\beta} - v_{\beta\alpha}).
\end{aligned}$$

Recall that for $A \in \Omega^1(\mathcal{M})$,

$$\mathcal{L} \circ (A, \nabla A) = -\frac{1}{4} F_{\mu\nu}F^{\mu\nu},$$

with $F = dA \in \Omega^2(\mathcal{M})$.

Now, consider the map $\Psi_f : \Omega^1(\mathcal{M}) \to \Omega^1(\mathcal{M})$, $\Psi_f(A) = A - df$, where $f \in C^\infty(\mathcal{M})$. Since $d\Psi_f(A) = dA = F$, it follows immediately that:

$$\mathcal{L} \circ (\Psi_f(A), \nabla\Psi_f(A)) = \mathcal{L} \circ (A, \nabla A).$$[17]

[16] This is called the Belinfante–Rosenfeld modification.

[17] Exercise: Determine the corresponding Noether currents.

The maps Ψ_f are called a *gauge transformations*. Below, we will show that they can be associated to a Lie group (a *gauge group*) by adding another field to the electromagnetic Lagrangian. We consider (ϕ, A), with $\phi \in C^\infty(\mathcal{M};\mathbb{C})$ and $A \in \Omega^1(\mathcal{M})$. Fix $f \in C^\infty(\mathcal{M})$. Consider the maps:

$$\begin{aligned}\Phi_f : C^\infty(\mathcal{M};\mathbb{C}) \times \Omega^1(\mathcal{M}) &\to C^\infty(\mathcal{M};\mathbb{C}) \times \Omega^1(\mathcal{M}),\\ \Phi_f(A,\phi)(x) &= (A(x) - df(x), e^{i\mathfrak{e}f(x)}\phi(x)),\end{aligned}$$

with $\mathfrak{e} \in \mathbb{R}$ arbitrary. In slight abuse of notation, we will also denote $\Phi_f(\phi)(x) = e^{i\mathfrak{e}f(x)}\phi(x)$ and $\Phi_f(A) = A - df$.

We wish to combine the electromagnetic Lagrangian with the Lagrangian from Example 3.8 with $\mathfrak{m} = 0$, such that the resulting Lagrangian is invariant under Φ_f ("gauge invariant"). For this purpose, we introduce the following operator:

$$\begin{aligned}d^A &: C^\infty(\mathcal{M};\mathbb{C}) \to \Omega^1(\mathcal{M};\mathbb{C})\\ d^A\phi &= d\phi + i\mathfrak{e}\phi A,\end{aligned}$$

with $\mathfrak{e} \in \mathbb{R}$.

Proposition 4.1. *Consider the Lagrangian:*

$$\begin{aligned}\mathcal{L} &: \mathcal{N} \to \mathbb{R}, \quad \text{with}\\ \mathcal{N} &= \coprod_{x\in\mathcal{M}} \mathbb{C} \times (T_x^*\mathcal{M} \otimes \mathbb{C}) \times \wedge^1 T_x^*\mathcal{M} \times (T_x^*\mathcal{M} \otimes \wedge^1 T_x^*\mathcal{M})\\ \mathcal{L}(x,q,p,v,w) &= \underbrace{\frac{1}{2}(g^{-1})_x^{\mu\nu} v_\mu \overline{v}_\nu}_{\text{"scalar field part"}} - \underbrace{\frac{1}{4}(g^{-1})_x^{\alpha\mu}(g^{-1})_x^{\beta\nu}(w_{\mu\nu} - w_{\nu\mu})(w_{\alpha\beta} - w_{\beta\alpha})}_{\text{"electromagnetic part"}}.\end{aligned}$$

Then

$$\mathcal{L} \circ (\phi, A, d^A\phi, \nabla A) = \mathcal{L} \circ (\Phi_f(\phi, A), d^{\Phi_f(A)}\Phi_f(\phi), \nabla\Phi_f(A)).$$

Proof. We will show that $d^A\Phi_f(\phi)(x) = e^{i\mathfrak{e}f(x)}d^A\phi(x)$.

$$\begin{aligned}d_\mu^{\Phi_f(A)}\Phi_f(\phi) &= d_\mu^A(e^{i\mathfrak{e}f}\phi) = \partial_\mu(e^{i\mathfrak{e}f}\phi) + i\mathfrak{e}\Phi_f(A)_\mu e^{if}\phi\\ &= e^{i\mathfrak{e}f}\partial_\mu\phi + i\mathfrak{e}\partial_\mu f e^{i\mathfrak{e}f}\phi + i\mathfrak{e}(A_\mu - \partial_\mu f)e^{i\mathfrak{e}f}\phi\\ &= e^{i\mathfrak{e}f}(\partial_\mu\phi + i\mathfrak{e}\phi A_\mu)\\ &= e^{i\mathfrak{e}f}d_\mu^A\phi.\end{aligned}$$

Hence,

$$(g^{-1})^{\mu\nu}d_\mu^{\Phi_f(A)}\Phi_f(\phi)\overline{d_\nu^{\Phi_f(A)}\Phi_f(\phi)} = (g^{-1})^{\mu\nu}d^A\phi_\mu\overline{d^A\phi_\nu}.$$

We already showed that $d\Phi_f(A) = dA = F$, so the electromagnetic part of the Lagrangian is also invariant under Φ_f. □

We can interpret the map $\Phi_f : C^\infty(\mathcal{M};\mathbb{C}) \to C^\infty(\mathcal{M};\mathbb{C})$, $\Phi_f(\phi)$, as a group action corresponding to the Lie group $U(1)$ at each $x \in \mathbb{R}^{n+1}$. Indeed, if we identify $\mathbb{R}^2$ with $\mathbb{C}$, we can express

$$U(1) = \{z \in \mathbb{C} \,|\, |z| = 1\},$$

so $z = e^\theta$, where $\theta \in i\mathbb{R} \cong \mathfrak{u}(1)$. Consider the map

$$\begin{aligned}\Phi &: C^\infty(\mathcal{M};U(1)) \times C^\infty(\mathbb{R}^{n+1};\mathbb{C}) \to \mathbb{C}^\infty(\mathbb{R}^{n+1};\mathbb{C}),\\ \Phi(g,\phi)(x) &= g(x)\phi(x).\end{aligned}$$

Note that $\Phi(gh,\phi)(x) = \Phi(g,\Phi_h(\phi))(x)$ and $\Phi(e,\phi) = \phi$, so Φ is a left group action.

We have that $\Phi(g,\phi) = \Phi_f(\phi)$, for $f \in C^\infty(\mathcal{M})$ such that $e^{i\mathfrak{e}f} = g$.

4.2 Gauge transformations for Lie groups

The above characterization of gauge transformations as group actions corresponding to a Lie group provides a path towards generalizing gauge transformations in the context of more general Lie groups.

In this section, we will assume that $\mathcal{M}$ is an $n+1$ dimensional manifold that is covered by a single coordinate chart. For example, we could consider $\mathcal{M} = \mathbb{R}^{n+1}$ in Cartesian coordinates. Equivalently, we could restrict to $U \subset \mathcal{M}$ covered by a single chart. This is implicitly done in most physics texts. It is possible to introduce all the notions below more generally outside the domain of a single coordinate chart, but this requires more advanced geometric notions like *principal G-bundles* and *adjoint bundles*.

Definition 4.1. *Let G be a Lie group of dimension m and V a finite-dimensional vector space. Then a* representation *of G is a smooth group homomorphism*[18]*:*

$$\Pi : G \to GL(V).$$

The derivative map of Π at the identity $\pi : \mathfrak{g} \cong T_eG \to \mathfrak{gl}(V)$ then defines a representation *of the associated Lie algebra $\mathfrak{g}$, which a Lie algebra homomorphism, i.e. a linear map:*

$$\pi : \mathfrak{g} \to \mathfrak{gl}(V),$$

such that $\pi([X,Y]) = \rho(X)\rho(Y) - \rho(Y)\rho(X)$ for all $X, Y \in \mathfrak{g}$.

We can express:

$$\pi(X) = \frac{d}{ds}|_{s=0}\Pi(\exp(sX)),$$

where $\exp : \mathfrak{gl}(V) \to GL(V)$ is the (matrix) exponential map.

Let $\phi \in C^\infty(\mathcal{M}; V)$. Then

$$\begin{aligned} \Phi : C^\infty(\mathcal{M}; G) \times C^\infty(\mathcal{M}; V) &\to C^\infty(\mathcal{M}; V), \\ \Phi(g, \phi)(x) &= \Pi(g(x))\phi(x) \end{aligned}$$

is a left-group action. Denote $\Phi_g = \Phi(g, \cdot) : C^\infty(\mathcal{M}; V) \to C^\infty(\mathcal{M}; V)$.

Definition 4.2. *Let $\mathcal{M}$ be a manifold, G a Lie group, V a vector space and $\mathfrak{g}$ the associated Lie algebra. Let $A \in \Omega^1(\mathcal{M}; \mathfrak{g})$ and $\phi \in C^\infty(\mathcal{M}; V)$.*

Then the covariant derivative associated to (G, Π, A) on $(\mathcal{M}, g)$ *is the following map:*

$$\begin{aligned} d^A : C^\infty(\mathcal{M}; V) &\to \Omega^1(\mathcal{M}; V), \\ d^A\phi &= d\phi + \pi(A)\phi, \end{aligned}$$

where $\pi(A) \in \Omega^1(\mathcal{M}; \mathfrak{gl}(V)) = \Gamma(\mathfrak{gl}(V) \otimes T^*\mathcal{M})$ defined as follows: $\pi(A) = \pi(e_i) \otimes A^i$, with e_i, $i = 1, \ldots, \dim G$ a basis of $\mathfrak{g}$.

An important class of Lie groups are matrix Lie groups. They are the main Lie groups that play a role in physics.

Definition 4.3. *A matrix Lie group G is a subgroup of $GL(m)$ ($m \times m$ invertible matrices) or $GL(m; \mathbb{C})$ ($m \times m$ invertible matrices with complex entries) such that G is topologically closed in $GL(m)$.*

Example 4.1. *Let G be a matrix Lie group such that $G \subset GL(V)$, for some finite dimensional vector space V. Then the fundamental representation is defined as $\Pi : G \to GL(V)$ with $\Pi(g) = g$ and the corresponding Lie algebra representation is $\pi : \mathfrak{g} \to \mathfrak{gl}(V)$, with $\pi(X) = X$. The corresponding covariant derivative then takes the form:*

$$d^A\phi = d\phi + A\phi = d\phi + e_i(\phi) \otimes A^i.$$

[18] This means: $\Pi(gh) = \Pi(g)\Pi(h)$ for all $g, h \in G$.

Example 4.2. *Let G be a Lie group. Consider the conjugation maps $\Psi^g : G \to G$, $\Psi^g(h) = ghg^{-1}$ and their derivative maps at the identity $d\Psi^g_e : T_eG \to T_eG$. Then $\mathrm{Ad} : g \mapsto d\Psi^g_e$ defines a Lie group representation with $V = T_eG \cong \mathfrak{g}$. We denote $\mathrm{Ad}_g = \mathrm{Ad}(g)$. Furthermore, if G is a matrix Lie group, then $\mathrm{Ad}(g)(X) = gXg^{-1}$. (*Exercise*)*

*It can be shown (*Exercise*) that the adjoint representation of the corresponding Lie algebra $\mathfrak{g}$ then satisfies: for all $X, Y \in \mathfrak{g}$*

$$\mathrm{ad} : \mathfrak{g} \to \mathfrak{gl}(\mathfrak{g}),$$
$$\mathrm{ad}(X)(Y) = [X, Y].$$

One can directly verify that ad *is a Lie algebra homomorphism by applying the Jacobi identity:*

$$\mathrm{ad}([X,Y])(Z) = [[X,Y],Z] = -[[Y,Z],X] - [[Z,X],Y] = [X,[Y,Z]] - [Y,[X,Z]] = \mathrm{ad}(Y)\mathrm{ad}(X)(Z) - \mathrm{ad}(X)\mathrm{ad}(Y)(Z).$$

The corresponding covariant derivative of $\phi \in C^\infty(\mathcal{M}; \mathfrak{g})$ is given by:

$$d^A\phi = d\phi + \mathrm{ad}(A)\phi = d\phi + [A, \phi] := d\phi + [e_i, \phi] \otimes A^i.$$

In order to define a gauge transformation for a pair (ϕ, A) we still need to find a transformation $\Phi_g(A)$ of $A \in \Omega^1(\mathcal{M}; \mathfrak{g})$, with $g \in C^\infty(\mathcal{M}; G)$, that guarantees that

$$d^{\Phi_g(A)}(\Phi_g\phi)(x) = \Pi(g(x))(d^A\phi)(x),$$

which is analogous to what we saw for $G = U(1)$.

Proposition 4.2. *Let G be a compact and connected matrix Lie group. Let $g \in C^\infty(\mathcal{M}; G)$. The map*

$$\Phi_g : \Omega^1(\mathcal{M}; \mathfrak{g}) \to \Omega^1(\mathcal{M}; \mathfrak{g}),$$
$$\Phi_g(A)(x) = \mathrm{Ad}_{g(x)}(A(x)) - \partial_\mu g(x) g^{-1}(x) \otimes dx^\mu = g(x) e_i g^{-1}(x) \otimes A^i - \partial_\mu g(x) g^{-1}(x) \otimes dx^\mu$$

is well-defined and for all $\phi \in C^\infty(\mathcal{M}; V)$

$$d^{\Phi_g(A)}(\Phi_g(\phi))(x) = \Pi(g(x))(d^A\phi)(x).$$

We refer to Φ_g as a (local) gauge transformation.

Remark 4.1. *Note that the transformation in Proposition 4.2 only makes sense in the domain of a coordinate chart and for G a matrix Lie group. Recall that on the abelian group $G = U(1)$, we had $\Phi_g(A) = A - df$ which does make sense globally.*

We first prove the following lemma:

Lemma 4.3. *Consider (G, Π), with G a connected and compact Lie group and Π a Lie group representation. Let $\mathfrak{g}$ be the corresponding Lie algebra.*

(i) *If $X \in \mathfrak{g}$ and $g \in G$, then*
$$\pi(X) = \Pi(g^{-1})\pi(\mathrm{Ad}_g(X))\Pi(g).$$

(ii) *Let G be a matrix Lie group and $\gamma : I \to G$ a smooth curve. Then*
$$\frac{d\gamma}{ds}(s)\gamma(s)^{-1} \in \mathfrak{g}$$
and
$$\frac{d}{ds}\left(\Pi(\gamma)\right)(s)\Pi(\gamma(s)^{-1}) = \pi\left(\frac{d\gamma}{ds}(s)\gamma(s)^{-1}\right).$$

(iii) *Let $g \in C^\infty(\mathcal{M}; G)$, with G a matrix Lie group. Then for all $0 \le \mu \le n+1$ and $x \in \mathcal{M}$, $\partial_\mu g(x) g(x)^{-1} \in \mathfrak{g}$ and*
$$\partial_\mu(\Pi \circ g)(x)(\Pi(g(x)))^{-1} = \pi(\partial_\mu g(x) g(x)^{-1}).$$

Proof. Let $g \in G$. Note that there always exists a $\theta \in \mathfrak{g}$, such that $g = \exp(\theta)$, if $\exp : \mathfrak{g} \to G$ is surjective. A sufficient condition for surjectivity turns out out to be connectedness and compactness for G. Then $\Pi(g) = \exp(\pi(\theta))$ and $\Pi(g^{-1}) = \exp(-\pi(\theta))$, so

$$\Pi(g^{-1})\pi(\mathrm{Ad}_g(X))\Pi(g) = \exp(-\pi(\theta))\pi(\mathrm{Ad}_{\exp(\theta)}(X))\exp(\pi(\theta)).$$

We consider $f : I \to \mathfrak{g}$, with $I \subset \mathbb{R}$ a neighbourhood of 0 and

$$f(s) = \exp(-\pi(s\theta))\pi(\mathrm{Ad}_{\exp(s\theta)}(X))\exp(\pi(s\theta)).$$

Then $f(0) = \pi(X)$. We will show that $f'(s) = 0$ to conclude (i).

Since $\mathrm{Ad}_{gh}(X) = \mathrm{Ad}_g(\mathrm{Ad}_h(X))$ for all $g, h \in G$, we can write

$$\frac{d}{ds}|_{s=s_0}\mathrm{Ad}_{\exp(s\theta)}(X) = \frac{d}{ds}|_{s=0}(\mathrm{Ad}_{\exp(s\theta)}(\mathrm{Ad}_{\exp(s_0\theta)}(X)) = \mathrm{ad}_\theta(\mathrm{Ad}_{\exp(s_0\theta)}(X)) = [\theta, \mathrm{Ad}_{\exp(s_0\theta)}(X)].$$

We have that by the product rule and linearity of π:

$$\begin{aligned} f'(s_0) = \exp(-s_0\pi(\theta))\Big(&- \pi(\theta)\pi(\mathrm{Ad}_{\exp(s_0\theta)}(X)) + \pi(\mathrm{Ad}_{\exp(s_0\theta)}(X))\pi(\theta) \\ &+ \pi([\theta, \mathrm{Ad}_{\exp(s_0\theta)}(X)])\Big)\exp(s_0\pi(\theta)) \\ = \exp(-s_0\pi(\theta)\Big(&- [\pi(\theta), \pi(\mathrm{Ad}_{\exp(s_0\theta)}(X))] + \pi([\theta, \mathrm{Ad}_{\exp(s_0\theta)}(X)])\Big) \\ = 0. \end{aligned}$$

This concludes (i).

We now turn to (ii). Let $s_0 \in I$. Define $\rho : I \to G$ as follows: $\rho(s) = \gamma(t + s_0)\gamma(s_0)^{-1}$. Then $\rho(0) = e$, so $\rho'(0) \in \mathfrak{g}$. Since we can express

$$\rho'(0) = \gamma'(s_0)\gamma(s_0)^{-1},$$

we have that $\gamma'(s_0)\gamma(s_0)^{-1} \in \mathfrak{g}$ for all $s_0 \in I$. Furthermore, we can express:

$$\frac{d}{ds}|_{s=s_0}\left(\Pi(\gamma)\right)(s)\Pi(\gamma^{-1}(s_0)) = \frac{d}{ds}|_{s=s_0}\left(\Pi(\rho(s)\gamma(s_0))\right)(s_0)\Pi(\gamma^{-1}(s_0)) = (\Pi \circ \rho)'(0).$$

We also have that

$$\pi\left(\frac{d\gamma}{ds}(s_0)\gamma^{-1}(s_0)\right) = \pi(\rho'(0)).$$

By definition of the Lie algebra representation,

$$\pi(\rho'(0)) = \frac{d}{ds}|_{s=0}\Pi(\exp(t\rho'(0))) = \frac{d}{ds}|_{s=0}\Pi(\rho)(s) = (\Pi \circ \rho)'(0).$$

This gives the desired identity.

We obtain (iii) by letting $\gamma(s) = g(\delta(s))$, with $\delta : I \to \mathcal{M}$, $\delta(s_0) = x$ and $\delta'(s_0) = \partial_\mu|_x$. Then $\gamma'(s_0) = \partial_\mu g(x)$ and applying (ii) at $s = s_0$. □

Proof of Proposition 4.2. By Lemma 4.3, the map Φ_g is well-defined. We denote with $\Pi(g)$ the map $x \mapsto \Pi(g(x))$. We can write locally, in the domain of a chart:

$$\begin{aligned} d^{\Phi_g(A)}\Pi(g)(\phi(x)) &= d(\Pi(g)\phi)(x) + \pi\left(\mathrm{Ad}_{g(x)}(A_\mu) - \partial_\mu g(x)g^{-1}(x)\right)\Pi(g)\phi(x) \otimes dx^\mu \\ &\overset{\text{(i) of Lemma 4.3}}{=} \Pi(g(x))\left(d\phi(x) + \pi(A_\mu(x))\phi(x)\right) \otimes dx^\mu + \partial_\mu\Pi(g)(x)\phi(x) \otimes dx^\mu - \pi(\partial_\mu g(x)g^{-1}(x))\Pi(g)\phi(x) \otimes dx^\mu \\ &\overset{\text{(iii) of Lemma 4.3}}{=} \Pi(g(x))\left(d\phi(x) + \pi(A_\mu(x))\phi(x)\right) \otimes dx^\mu + \partial_\mu\Pi(g)(x)\phi(x) \otimes dx^\mu - \partial_\mu\Pi(g)(x)\phi(x) \otimes dx^\mu \\ &= \Pi(g)(x)\left(d\phi(x) + \pi(A_\mu(x))\phi(x) \otimes dx^\mu\right) = \Pi(g(x))(d^A\phi(x)). \end{aligned}$$

To obtain the third identity, we moreover used that $\partial_\mu g(x) = \frac{d}{ds}(g \circ \gamma)(0)$, where $\gamma(0) = x$ and $\gamma'(0) = \partial_\mu$, and then applied (ii) of Lemma 4.3 to the curve $s \mapsto (g \circ \gamma)(s)$. □

Definition 4.4. *Let G be a connected and compact matrix Lie group, V a finite-dimensional vector space and Π the corresponding Lie group representation. Let $g \in C^\infty(\mathcal{M}; G)$. Then a (local) gauge transformation corresponding to (G, V, Π) is defined as follows:*

$$\Phi_g : C^\infty(\mathcal{M}; V) \times \Omega^1(\mathcal{M}; \mathfrak{g}) \to C^\infty(\mathcal{M}; V) \times \Omega^1(\mathcal{M}; \mathfrak{g}),$$
$$\Phi_g(\phi, A)(x) = \Big(\Pi(g(x))\phi(x), \mathrm{Ad}_{g(x)}(A(x)) - \partial_\mu g(x) g(x)^{-1} \otimes dx^\mu\Big).$$

4.3 Yang–Mills theory

In this section, we will construct gauge invariant Lagrangians corresponding to connected, compact matrix Lie groups G. As in the previous section, we will assume that $\mathcal{M}$ is covered by a single coordinate chart.

We will first extend the covariant derivative d^A to $\Omega^r(\mathcal{M}; \mathfrak{g})$.

Definition 4.5. *Let $\theta \in \Omega^s(\mathcal{M}; \mathfrak{g})$ and $\omega \in \Omega^r(\mathcal{M}; \mathfrak{g})$. Then we define the wedge product of $\mathfrak{g}$-valued differential forms as follows:*

$$[\theta \wedge \omega] := [e_i, e_j] \otimes \theta^i \wedge \omega^j \in \Omega^{r+s}(\mathcal{M}; \mathfrak{g}).$$

Definition 4.6. *Let $A \in \Omega^1(\mathcal{M}; \mathfrak{g})$ and $\omega \in \Omega^r(\mathcal{M}; \mathfrak{g})$ with $r \geq 1$. Then we define the covariant derivative d^A associated to the adjoint representation as follows:*

$$d^A : \Omega^r(\mathcal{M}; \mathfrak{g}) \to \Omega^{r+1}(\mathcal{M}; \mathfrak{g}),$$
$$d^A\omega = d\omega + [A \wedge \omega],$$

With respect to a coordinate chart, we have that for $\omega \in \Omega^r(\mathcal{M}; \mathfrak{g})$:

$$\begin{aligned}(d^A\omega)_{\mu\mu_1\ldots\mu_r} &= (r+1)\nabla_{[\mu}\omega_{\mu_1\ldots\mu_r]} + [e_i, e_j](A^i \wedge \omega^j)_{\mu\mu_1\ldots\mu_r} \\ &= (r+1)\nabla_{[\mu}\omega_{\mu_1\ldots\mu_r]} + \frac{(r+1)!}{r!}[e_i, e_j]A^i_{[\mu}\omega^j_{\mu_1\ldots\mu_r]} \\ &= (r+1)\Big(\nabla_{[\mu}\omega_{\mu_1\ldots\mu_r]} + [A_{[\mu}, \omega_{\mu_1\ldots\mu_r]}]\Big)\end{aligned}$$

Definition 4.7. *Let $\mathcal{M}$ be a manifold and let G be a Lie group with Lie algebra $\mathfrak{g}$. Let d^A denote the covariant derivative associated to the adjoint representation. Then the* Yang–Mills field strength $F \in \Omega^2(\mathcal{M}; \mathfrak{g})$ *corresponding to G is defined as follows:*

$$F = dA + \frac{1}{2}[A \wedge A],$$

or, locally,

$$F = (\partial_\mu A_\nu - \partial_\nu A_\mu) \otimes dx^\mu \otimes dx^\nu + [A_\mu, A_\nu] \otimes dx^\mu \otimes dx^\nu.$$

In contrast with partial derivatives, the covariant derivatives d^A associated to (G, Π, A) do not commute. We show below that the Yang–Mills field strength corresponds to their commutator.

Proposition 4.4. *Let $\omega \in \Omega^r(\mathcal{M}; \mathfrak{g})$. Then*

$$d^A d^A \omega = [F \wedge \omega].$$

In particular, with respect to any coordinate chart:

$$d^A_\mu d^A_\nu \phi - d^A_\nu d^A_\mu \phi = (d^A d^A \phi)_{\mu\nu} = [F_{\mu\nu}, \phi].$$

Proof. We have that

$$\begin{aligned}d^A(d^A\omega) = d^A\left(d\omega + [A \wedge \omega]\right) &= d^2\omega + [dA \wedge \omega] - [A \wedge d\omega] + [A \wedge d\omega] + \overbrace{[A \wedge [A \wedge \omega]]}^{=\frac{1}{2}[[A\wedge A]\wedge\omega]} \\ &= \left[\left(dA + \frac{1}{2}[A \wedge A]\right) \wedge \omega\right] = [F \wedge \omega],\end{aligned}$$

where we used that by the Jacobi identity:

$$\begin{aligned}[A \wedge [A \wedge \omega]] &= [e_i, [e_j, e_k]] \otimes A^i \wedge A^j \wedge \omega^k \\ &= -[e_j, [e_k, e_i]] \otimes A^i \wedge A^j \wedge \omega^k - [e_k, [e_i, e_j]] \otimes A^i \wedge A^j \wedge \omega^k \\ &= -[e_j, [e_i, e_k]] \otimes A^j \wedge A^i \wedge \omega^k + [[e_i, e_j], e_k] \otimes A^i \wedge A^j \wedge \omega^k \\ &= -[A \wedge [A \wedge \omega]] + [[A \wedge A] \wedge \omega].\end{aligned}$$

□

Proposition 4.5. *Let $\Phi_g : \Omega^1(\mathcal{M}; \mathfrak{g}) \to \Omega^1(\mathcal{M}; \mathfrak{g})$ be the gauge transformation from Proposition 4.2. Write*

$$F^{\Phi_g(A)} = d\Phi_g(A) + \frac{1}{2}[\Phi_g(A) \wedge \Phi_g(A)].$$

Then, locally,

$$F^{\Phi_g(A)} = g(x)F_{\mu\nu}(x)g^{-1} \otimes dx^\mu \otimes dx^\nu = g(x)e_i(x)g^{-1}(x) \otimes F^i(x).$$

Proof. We will use that

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu].$$

Let $g \in C^\infty(\mathcal{M}; G)$. Observe that $0 = \partial_\mu(gg^{-1}) = (\partial_\mu g)g^{-1} + g\partial_\mu g^{-1}$, so $\partial_\mu g^{-1} = -g^{-1}(\partial_\mu g)g^{-1}$, from which it follows that

$$\begin{aligned}(F^{\Phi_g(A)})^i_{\mu\nu} &= \Big(\partial_\mu(gA_\nu g^{-1} - (\partial_\nu g)g^{-1}) - \partial_\nu(gA_\mu g^{-1} - (\partial_\mu g)g^{-1}\Big) \\ &\quad + [gA_\mu g^{-1} - (\partial_\mu g)g^{-1}, gA_\nu g^{-1} - (\partial_\nu g)g^{-1}] \\ &= g(\partial_\mu A_\nu - \partial_\nu A_\mu)g^{-1} + g[A_\mu, A_\nu]g^{-1} + (\partial_\mu g)A_\nu g^{-1} - (\partial_\nu g)A_\mu g^{-1} \\ &\quad - (gA_\nu g^{-1})(\partial_\mu g)g^{-1} + (gA_\mu g^{-1})(\partial_\nu g)g^{-1} \\ &\quad - \partial_\nu g\partial_\mu g^{-1} + \partial_\mu g\partial_\nu g^{-1} \\ &\quad - gA_\mu g^{-1}(\partial_\nu g)g^{-1} - (\partial_\mu g)A_\nu g^{-1} \\ &\quad + gA_\nu g^{-1}(\partial_\mu g)g^{-1} + (\partial_\nu g)A_\mu g^{-1} \\ &\quad + \underbrace{(\partial_\mu g)g^{-1}(\partial_\nu g)g^{-1} - (\partial_\nu g)g^{-1}(\partial_\mu g)g^{-1}}_{=-(\partial_\mu g)\partial_\nu g^{-1} + \partial_\nu g\partial_\mu g^{-1}} \\ &= gF_{\mu\nu}g^{-1}.\end{aligned}$$

□

In order to construct a gauge invariant Lagrangian, we still need a way of combining components of F to obtain a real-valued function.

Definition 4.8. *The Killing form $B : \mathfrak{g} \times \mathfrak{g} \to \mathbb{R}$ is a symmetric bilinear form defined as follows:*

$$B(X, Y) = \mathrm{tr}(\mathrm{ad}\,(X)\mathrm{ad}\,(Y)).$$

Remark 4.2. *A simply connected Lie group G is* semisimple *if and only if the Killing form κ is non-degenerate. The Killing form of a compact, semisimple Lie group is negative definite.*

Lemma 4.6. *Let G be a matrix Lie group with Lie algebra $\mathfrak{g}$. Let $X, Y \in \mathfrak{g}$ and $g \in G$. Then*

$$B(gXg^{-1}, gYg^{-1}) = B(X, Y).$$

Proof. By (i) of Lemma 4.3, we have that

$$\mathrm{ad}(gXg^{-1}) = \mathrm{Ad}(g)\mathrm{ad}(X)\mathrm{Ad}(g^{-1}).$$

Then, by the cyclic property of the trace,

$$\begin{aligned}B(gXg^{-1}, gYg^{-1}) &= \mathrm{tr}(\mathrm{ad}\,(gXg^{-1})\mathrm{ad}\,(gYg^{-1})) = \mathrm{tr}(\mathrm{Ad}\,(g)\mathrm{ad}\,(X)\mathrm{Ad}\,(g^{-1})\mathrm{Ad}\,(g)\mathrm{ad}\,(Y)\mathrm{Ad}\,(g^{-1})) \\ &= \mathrm{tr}(\mathrm{ad}\,(X)\mathrm{ad}\,(Y)) = B(X, Y).\end{aligned}$$

□

Now we define the Yang–Mills Lagragian.

Definition 4.9. *Let G be a semisimple and compact matrix Lie group. Then the Yang–Mills Lagrangian is defined as follows:*

$$\begin{aligned}\mathcal{L}_{YM} &: \mathcal{N}_{YM} \to \mathbb{R},\\ \mathcal{N}_{YM} &= \coprod_{x\in\mathcal{M}} T_x^*\mathcal{M}\otimes\mathfrak{g}\times\wedge^2(T_x^*\mathcal{M})\otimes\mathfrak{g},\\ \mathcal{L}_{YM}(x,q,v) &= -\frac{1}{4\mathfrak{e}^2}B\Big(v_{\alpha\beta}-v_{\beta\alpha}+[q_\alpha,q_\beta],v_{\mu\nu}-v_{\nu\mu}+[q_\mu,q_\nu]\Big)(g^{-1})_x^{\alpha\mu}(g^{-1})_x^{\beta\nu}.\end{aligned}$$

The fields are $A\in\Omega^1(\mathcal{M};\mathfrak{g})$ and the corresponding Yang–Mills action *is then given by:*

$$\mathcal{S}_{YM}(A) = -\frac{1}{4\mathfrak{e}^2}\int_{\mathcal{M}} B(e_i,e_j)\otimes(F^{\mu\nu})^i(F_{\mu\nu})^j\epsilon,$$

with F the Yang–Mills field strength corresponding to A.

Corollary 4.7. *The Yang–Mills Lagrangian is gauge invariant:*

$$\mathcal{L}_{YM}\circ(\Phi_g(A),\nabla\Phi_g(A)) = \mathcal{L}_{YM}\circ(A,\nabla A).$$

Proof. Combine Proposition 4.5 and Lemma 4.6. □

Remark 4.3. *We can get rid of the factor $\mathfrak{e}^{-2}$ by rescaling $A=\mathfrak{e}\hat{A}$, changing the covariant derivative to $d^{\hat{A}}=d+\mathfrak{e}\pi(\hat{A})\phi$ and the transformation of $\hat{A}$ to:*

$$\Phi_g(\hat{A})(x) = \mathrm{Ad}_{g(x)}(\hat{A}) - \mathfrak{e}^{-1}\partial_\mu g(x)g(x)^{-1}\otimes dx^\mu.$$

We leave it to the interested reader to derive the corresponding Euler–Lagrange equations, or *Yang–Mills equations*:

$$\nabla_\mu F^{\mu\nu} + [A_\mu, F^{\mu\nu}] = 0.$$

You will need the following associativity property of the Killing form: $B([X,Y],Z) = B(X,[Y,Z])$ for all $X,Y,Z\in\mathfrak{g}$ (Exercise).

F also satisfies (Exercise)

$$d^A F = 0.$$

In components, the above equation is equivalent to

$$(\partial_\mu F_{\nu\rho}+[A_\mu,F_{\nu\rho}])+(\partial_\nu F_{\rho\mu}+[A_\nu,F_{\rho\mu}])+(\partial_\rho F_{\mu\nu}+[A_\rho,F_{\mu\nu}])=0$$

and is called the *Bianchi identity*. We will encounter the analogue of this identity when we study the curvature properties of $(\mathcal{M},g)$.

Remark 4.4. *The standard model revolves around the Yang–Mills Lagrangian with $G=U(1)\times SU(2)\times SU(3)$ where the $U(1)\times SU(2)$ part describes the electroweak interaction (electromagnetism unified with weak nuclear interaction, the latter which is responsible for radioactive decay) and $SU(3)$ describes the strong nuclear interaction, which is responsible for binding quarks and neutrons and protons together in atomic nuclei).*

5 Quantum mechanics

5.1 The kinematic postulates of quantum mechanics

Recall the definition of a Hilbert space.

Definition 5.1. *A Hilbert space* $(\mathbf{H}, \langle\ ,\ \rangle)$ *is a vector space* $\mathbf{H}$ *equipped with an inner product* $\langle\ ,\ \rangle$*, which is a* sesquilinear form *on* $\mathbf{H}$*, i.e.* $\langle\ ,\ \rangle : \mathbf{H} \times \mathbf{H} \to \mathbb{C}$ *satisfies*

$$\langle x, \lambda y + z\rangle = \lambda\langle x, y\rangle + \langle x, z\rangle \quad \forall x, y, z \in \mathbf{H},\ \forall \lambda \in \mathbb{C},$$
$$\langle \lambda x + z, y\rangle = \overline{\lambda}\langle x, y\rangle + \langle x, z\rangle \quad \forall x, y, z \in \mathbf{H},\ \forall \lambda \in \mathbb{C},$$

that is moreover symmetric

$$\langle x, y\rangle = \overline{\langle y, x\rangle} \quad \forall x, y \in \mathbf{H}$$

and positive-definite:

$$\langle x, x\rangle > 0 \quad \forall x \in \mathbf{H} \setminus \{0\}.$$

Furthermore, $\mathbf{H}$ *is complete with respect to the corresponding norm defined as follows:* $|x| = \sqrt{\langle x, x\rangle}$*. We will moreover assume all Hilbert spaces are separable.*[19]

We will consider linear maps on $\mathbf{H}$ (defined on dense subspaces).

Definition 5.2.

- *A* linear operator *is a linear map*

$$A : \mathcal{D}(A) \to \mathbf{H},$$

with $\mathcal{D}(A) \subseteq \mathbf{H}$ *a linear subspace. We refer to* A *as an* densely defined operator *if* $\mathcal{D}(A)$ *is dense.*

- *We say* A *is a* bounded linear operator *if*

$$||A|| := \sup_{\substack{x \in \mathcal{D}(A) \\ |x|=1}} |Ax| < \infty.$$

A linear operator that does not satisfy A *is said to be* unbounded*.*

- *The (Hermitian) adjoint operator* A^* *corresponding to an densely defined operator* A *is defined as follows: let*

$$\mathcal{D}(A^*) = \{\psi \in \mathbf{H} \,|\, \phi \mapsto \langle \psi, A\phi\rangle \text{ is a bounded linear functional on } \mathcal{D}(A)\}.$$

Then $A^* : \mathcal{D}(A^*) \to \mathbf{H}$ *is a linear map defined as follows:* $A^*\psi = \chi$*, where* $\chi \in \mathbf{H}$ *is uniquely determined by* $\langle \chi, \phi\rangle = \langle \psi, A\phi\rangle$ *for all* $\phi \in \mathcal{D}(A)$ *by the Riesz Representation Theorem.*

Densely defined bounded linear operators admit a unique extension $A : \mathbf{H} \to \mathbf{H}$ by the Bounded Linear Transformation (BLT) Theorem. Furthermore, $A : \mathbf{H} \to \mathbf{H}$ is bounded if and only if A is (sequentially) continuous: $A\psi_n \to A\psi$ for all sequences $\{\psi_n\}$ such that $\psi_n \to \psi$.

Exercise: If A is a densely defined bounded linear operator, then $A^* : \mathbf{H} \to \mathbf{H}$ is well-defined. We denote with $B(\mathbf{H})$ the space of bounded linear operators on $\mathbf{H}$.

In general, we do not know how big the set $\mathcal{D}(A^*)$ is. We certainly have that $0 \in \mathcal{D}(A^*)$, but the set need not be dense in $\mathbf{H}$.

Recall also:

Definition 5.3. *Let* $A : \mathbf{H} \supseteq \mathcal{D}(A) \to \mathbf{H}$ *be a linear operator. A number* $\lambda \in \mathbb{C}$ *belongs to* $\rho(A)$*, the* resolvent set *of* A*, if there exists a* $R \in B(\mathbf{H})$ *such that:*

1. *For all* $\psi \in \mathbf{H}$*,* $R\psi \in \mathcal{D}(A)$ *and* $(A - \lambda\mathbf{1})R\psi = \psi$*,*

[19] It can be shown, using Zorn's Lemma, that every Hilbert space admits an orthonormal basis. Exercise: If $\mathbf{H}$ is separable, show that every orthonormal basis must be countable. In practice, one can often construct a countable orthonormal basis explicitly (without appealing to Zorn's Lemma).

2. *For all* $\psi \in \mathcal{D}(A)$, $R(A - \lambda \mathbf{1})\psi = \psi$.

The operator R *is referred to as a* resolvent operator of A *and is denoted by* $(A - \lambda I)^{-1}$. *The complement* $\sigma(A) := \mathbb{C} \setminus \rho(A)$ *is called the* spectrum of A.

In these lectures, we will can mostly restrict our consideration to symmetric or self-adjoint operators, which are defined as follows:

Definition 5.4. *Let* $A : \mathbf{H} \supseteq \mathcal{D}(A) \to \mathbf{H}$ *be a linear operator.*

- A *is* symmetric *if*
$$\langle \psi, A\phi \rangle = \langle A\psi, \phi \rangle \quad \forall \psi, \phi \in \mathcal{D}(A).$$
- *Let* A *be densely defined. Then* A *is* self-adjoint *if* $\mathcal{D}(A) = \mathcal{D}(A^*)$ *and* $A = A^*$.
- *Let* A *be densely defined. Then* A *is* closeable, *if* $\overline{\mathcal{D}(A^*)} = \mathbf{H}$. *The* closure *of* A *is defined as* $\overline{A} := (A^*)^*$.
- *Let* A *be densely defined and symmetric, so it is closeable by Proposition 5.1. Then* A *is* essentially self-adjoint *if* $\overline{A}$ *is self-adjoint.*
- *Let* A *be densely defined. Then* A *is* closed *if the graph* $\mathcal{G}(A) = \{(\psi, \phi) \in \mathcal{D}(A) \times \mathbf{H} \ , \ \phi = A\psi\}$ *is closed in* $\mathbf{H} \times \mathbf{H}$.

Will see for densely defined symmetric operators $\mathcal{D}(A) \subseteq \mathcal{D}(\overline{A})$. In practice, we are often given a symmetric operator on a dense domain and we consider the self-adjoint operator $\overline{A}$. In the physics literature, symmetry and self-adjointness are often mixed up and a symmetric/self-adjoint operator is sometimes called a "Hermitian operator".

The following properties of symmetric operators will be important for identifying probability within quantum mechanics.

Proposition 5.1. *Let* $A : \mathbf{H} \supseteq \mathcal{D}(A) \to \mathbf{H}$ *be a symmetric operator. Then:*

(i) $\langle \psi, A\psi \rangle \in \mathbb{R}$ *for all* $\psi \in \mathcal{D}(A)$. *Furthermore, for all* $m \in \mathbb{N}_1$, $\langle \psi, A^m\psi \rangle \in \mathbb{R}$ *if* $A^k\psi \in \mathcal{D}(A)$ *for all* $0 \leq k \leq m - 1$.

(ii) *Let* $\lambda \in \mathbb{C}$ *be an eigenvalue for* A, *i.e. there exists a* $\psi \in \mathcal{D}(A)$ *such that* $A\psi = \lambda\psi$. *Then* $\lambda \in \mathbb{R}$.

(iii) *Let* A *be self-adjoint. Then* $\sigma(A) \subseteq \mathbb{R}$.

(iv) *If* A *is densely defined, then* $\mathcal{D}(A) \subseteq \mathcal{D}(A^*)$ *and* $A = A^*$ *on* $\mathcal{D}(A)$, *so* A *is closeable. Furthermore,* $\mathcal{D}(A) \subseteq \mathcal{D}(\overline{A})$.

(v) *If* A *is densely defined, but not necessarily symmetric, then* A^* *is a closed operator. In particular, if* A *is closeable, then* $\overline{A}$ *is a closed operator.*

Proof. "(i)": By the symmetry property of inner products

$$\langle \psi, A\psi \rangle = \overline{\langle A\psi, \psi \rangle}.$$

By the symmetry of A:

$$\overline{\langle A\psi, \psi \rangle} = \overline{\langle \psi, A\psi \rangle}.$$

Hence, $\langle \psi, A\psi \rangle \in \mathbb{R}$.

Let $m \geq 1$ and $A^k\psi \in \mathcal{D}(A)$ for all $0 \leq k \leq m - 1$. Suppose m is even, then

$$\langle \psi, A^m\psi \rangle = \langle A^{\frac{m}{2}}\psi, A^{\frac{m}{2}}\psi \rangle = |A^{\frac{m}{2}}\psi|^2 \in \mathbb{R}.$$

Suppose m is odd. Then

$$\langle \psi, A^m\psi \rangle = \langle A^{\frac{m-1}{2}}\psi, AA^{\frac{m-1}{2}}\psi \rangle \in \mathbb{R},$$

by the fact that $\langle \phi, A\phi \rangle \in \mathbb{R}$ for all $\phi \in \mathcal{D}(A)$.

"(ii)": By (i) and sesquilinearity of the inner product:

$$\lambda|\psi|^2 = \langle \psi, \lambda\psi\rangle = \langle \psi, A\psi\rangle \in \mathbb{R}. \qquad \square$$

"(iii)": We omit the proof of (iii) and refer to the "maths part" of the lectures.

"(iv)": Let $\psi, \phi \in \mathcal{D}(A)$. Then $\langle A\psi, \phi\rangle = \langle \psi, A\phi\rangle$ by the symmetry of A. By Cauchy–Schwarz, we therefore have that

$$|\langle \psi, A\phi\rangle| = |\langle A\psi, \phi\rangle| \leq |A\psi||\phi|.$$

Hence, $\phi \mapsto \langle \psi, A\phi\rangle$ defines a bounded functional and therefore $\psi \in \mathcal{D}(A^*)$ and $A^*\phi = A\phi$. Since $\mathcal{D}(A) \subseteq \mathcal{D}(A^*)$ and $\mathcal{D}(A)$ is dense in $\mathbf{H}$, $\mathcal{D}(A^*)$ must also be dense in $\mathbf{H}$. Therefore $\overline{A} = (A^*)^*$ is well-defined, and by the above $\mathcal{D}(A^*) \subseteq \mathcal{D}(\overline{A})$.

"(v)": Let $\{\psi_n\}$ be a sequence in $\mathcal{D}(A^*)$, such that $\psi_n \to \psi$, $A^*\psi_n \to \phi$ in $\mathbf{H}$ as $n \to \infty$. To conclude that A^* is closed, we need to show that $\psi \in \mathcal{D}(A^*)$ and $A^*\psi = \phi$.

We have that for all $\chi \in \mathcal{D}(A)$,

$$\langle A^*\psi_n, \chi\rangle = \langle \psi_n, A\chi\rangle$$

an hence

$$\langle \phi, \chi\rangle = \lim_{n\to\infty} \langle A^*\psi_n, \chi\rangle = \lim_{n\to\infty} \langle \psi_n, A\chi\rangle = \langle \psi, A\chi\rangle.$$

From this it follows that the functional $\chi \mapsto \langle \psi, A\chi\rangle$ is bounded on $\mathcal{D}(A)$, so $\psi \in \mathcal{D}(A^*)$ and moreover $A^*\psi = \phi$. Since $\overline{A} = (A^*)^*$, we can apply the above argument to A^* instead of A to conclude that $\overline{A}$ is also closed.

EXERCISE: Let $A : \mathcal{D}(A) \to \mathbf{H}$ be densely defined and assume that A^* is an extension of A, i.e. $\mathcal{D}(A) \subseteq \mathcal{D}(A^*)$ and $A = A^*$ on $\mathcal{D}(A)$. Then A must be symmetric.

Symmetric bounded operators are self-adjoint. In general, (essential) self-adjointness implies symmetry, but the converse is not always true.

We will now list the main kinematic (i.e. non-dynamic) postulates of quantum mechanics and introduce some additional mathematical concepts along the way.

Postulate 1. *A* state of a physical system *is the following equivalence class of unit norm elements of a Hilbert space* $(\mathbf{H}, \langle\ ,\ \rangle)$*:*

$$[\psi] := \{\phi \in \mathbf{H},\ |\ \phi = c\psi,\ c \in \mathbb{C},\ |c| = 1\}.$$

In practice, one often refers to unit norm elements $\psi \in \mathbf{H}$ as states, but, as we will see when we define the measurement postulate, any ϕ such that $\phi = c\psi$ with $|c| = 1$ produces the same measurement results. Recall that in classical mechanics, a state of a 1-particle system in $\mathbb{R}^n$ is a point in phase space $\mathbb{R}^{2n}$.

Remark 5.1. *The above definition of a state is also called a "pure state" to distinguish it from a more general notion of state called a "mixed state", which we will define later.*

In the physics literature, you will often encounter the "Dirac bra-ket" notation, where $|\psi\rangle$ (a "ket") denotes $\psi \in \mathbf{H}$. The notation $\langle\phi|$ (a "bra") is used for a bounded linear functional $\phi \in \mathbf{H}^*$ and the notation $\langle\phi|\psi\rangle$ means $\phi(\psi)$. This notation is also used for the inner product $\langle\phi, \psi\rangle$, with ϕ identified with its dual element in $\mathbf{H}$. Furthermore, $|\psi\rangle\langle\phi|$ denotes a linear operator A on $\mathbf{H}$, with $A\tilde{\psi} = \phi(\tilde{\psi})\psi$.

Postulate 2. *To each "appropriate" function $f : \mathbb{R}^{2n} \to \mathbb{R}$ on the classical phase space $\mathbb{R}^{2n}$, we can associate a self-adjoint operator $\hat{f} : \mathbf{H} \supseteq \mathcal{D}(\hat{f}) \to \mathbf{H}$.*

In Hamiltonian mechanics, *observables* are represented by real-valued functions on the phase space $\mathbb{R}^{2n}$ (for example, describing N particles in $\mathbb{R}^3$ in classical mechanics, with $n = 3N$). In quantum mechanics, observables are instead represented by self-adjoint operators on Hilbert spaces.

As we will later see, for $\mathbf{H} = L^2(\mathbb{R}^n)$ the coordinates (x^i, p_i) on phase space correspond to operators $\hat{x}^i\psi = x^i\psi$ and $\hat{p}_i\psi = -i\hbar\frac{\partial}{\partial x^i}\psi$, when restricted to appropriate domains. These are both unbounded operators.

Remark 5.2. *Taking products of real-valued functions $f \cdot g$, which is commutative, corresponds to considering composition of operators $\hat{f}\hat{g}$, which is non-commutative, i.e. we could have $\hat{f}\hat{g} \neq \hat{g}\hat{f}$. There is therefore an* ordering ambiguity *when mapping real-valued functions to operators on Hilbert spaces. A particular choice of ordering is called a* quantization scheme.

The proposition below motivates why cannot restrict to operators with $\mathcal{D}(A) = \mathbf{H}$ if we want to consider unbounded operators like position and momentum.

Proposition 5.2. *Let $A : \mathbf{H} \supseteq \mathcal{D}(A) \to \mathbf{H}$ be a densely defined symmetric operator. If $\mathcal{D}(A) = \mathbf{H}$, then A must be bounded.*

Proof. By Proposition 5.1 (iv), $A = A^*$ on $\mathbf{H} = \mathcal{D}(A) \subseteq \mathcal{D}(A^*)$ by Proposition 5.1 (iv). By Proposition 5.1 (v), we moreover have that $A = A^*$ is closed. Now we can appeal to the Closed Graph Theorem, which states that *closed operators with closed domains must be bounded.* □

Postulate 3. *Consider an observable $\hat{f}$ corresponding to a function $f : \mathbb{R}^{2n} \to \mathbb{R}$. For a physical system in a state represented by $\psi \in \mathcal{D}(\hat{f})$, the result of the measurement of f is governed by a* probability measure *$\mu_\psi^{\hat{f}}$ and the corresponding expectation value $\int_{\mathbb{R}} x \, d\mu_\psi^{\hat{f}}(x) = \int_{\mathbb{R}} \mathrm{id}_{\mathbb{R}} \, d\mu_\psi^{\hat{f}}$ is given by*

$$\langle \hat{f} \rangle_\psi := \langle \psi, \hat{f}\psi \rangle.$$

And more generally, the n-th moment with respect to $\mu_\psi^{\hat{f}}$, $\int_{\mathbb{R}} x^m \, d\mu_\psi^{\hat{f}}(x)$, is given by: $\langle \hat{f}^m \rangle_\psi = \langle \psi, \hat{f}^m \psi \rangle$.

Suppose we prepare a large ensemble of independent physical systems to lie in the same state ψ and perform measurements of an observable f (like position, momentum or energy) on each system. By Postulate 3, the measurement values should approach a probability distribution, determined by ψ and f, with expectation value $\langle \hat{f} \rangle_\psi$. Hence measurements are allowed to behave in a *non-deterministic* manner.

The above postulate motivates the consideration of equivalence classes of vectors in $\mathbf{H}$ in Postulate 1, as for $\psi_1, \psi_2 \in \mathbf{H}$ with $\psi_2 = c\psi_1$, $|c| = 1$,

$$\langle \hat{f} \rangle_{\psi_2} = \langle \psi_2, \hat{f}\psi_2 \rangle = \langle c\psi_1, c\hat{f}\psi_1 \rangle = \overline{c}c \langle \psi_1, \hat{f}\psi_1 \rangle = \langle \hat{f} \rangle_{\psi_1},$$

so ψ_1 and ψ_2 are indistinguishable by measurements.

Example 5.1. *In the case $\mathbf{H} = L^2(\mathbb{R})$ the measurement of position x has the following expectation value:*

$$\langle \hat{x} \rangle_\psi = \langle \psi, x \cdot \psi \rangle_{L^2(\mathbb{R})} = \int_{\mathbb{R}} x |\psi|^2(x) \, dx.$$

Hence, $|\psi|^2$ defines a probability density function and the corresponding probability measure is given by:

$$\mu_\psi^{\hat{x}}(\Omega) = \int_\Omega |\psi|^2 \, dx,$$

for $\Omega \in \mathcal{B}_{\mathbb{R}}$, the Borel σ-algebra of $\mathbb{R}$.

Example 5.2. *Let $A : \mathcal{D}(A) \to \mathbf{H}$ be a self-adjoint operator with unit eigenvector $\psi \in \mathcal{D}(A)$, such that $A\psi = \lambda\psi$. We have that $A^m\psi = \lambda^m\psi$, so $A^m\psi \in \mathcal{D}(A)$ for all $m \in \mathbb{N}_0$. Then*

$$\langle A^m \rangle_\psi = \langle \psi, A^m\psi \rangle = \lambda^m |\psi|^2 = \lambda^m.$$

Note that the Dirac measure $\delta_\lambda : \mathcal{B}_{\mathbb{R}} \to \mathbb{R}$ satisfies also

$$\int_{\mathbb{R}} \mathrm{id}_{\mathbb{R}}^m \, d\delta_\lambda = \int_{\mathbb{R}} x^m d\delta_\lambda(x) = x^m|_{x=\lambda} = \lambda^m.$$

Hence, in this case $\mu_\psi^A = \delta_\lambda$. It can even be shown that δ_λ is the unique *probability measure with $\langle A^m \rangle_\psi = \lambda^m$, but this lies outside the scope of this course.*

Example 5.3. *Let $A : \mathcal{D}(A) \to \mathbf{H}$ be a self-adjoint operator, such that $\mathcal{D}(A)$ has an orthonormal basis of eigenvectors $\{e_i\}_{i\in I}$ with distinct eigenvalues λ_i. Let $\psi \in \mathcal{D}(A)$, such that $A^m\psi \in \mathcal{D}(A)$ for all $m \in \mathbb{N}_0$. We can express $\psi = \sum_{i\in I} a_i e_i$, with $a_i \in \mathbb{C}$. The probability measure $\mu_\psi^A = \sum_{i\in I} |a_i|^2 \delta_{\lambda_i}$ results in the expectation value $\langle \hat{f} \rangle_\psi$, since*

$$\langle \psi, A^m\psi \rangle = \left\langle \sum_{j\in I} a_j \lambda_j^m e_j, \sum_{i\in I} a_i \lambda_i^m e_i \right\rangle = \sum_{i\in I} |a_i|^2 \lambda_i^m.$$

More generally, the *Spectral Theorem* provides a canonical way of assigning a probability measure μ_ψ^A on $\mathcal{B}_\mathbb{R}$ to a self-adjoint operator that is consistent with the expectation values $\langle A^m \rangle_\psi$.

To understand the formulation of the Spectral Theorem, we first define the notion of a *projection-valued measure* or PVM.

Definition 5.5. *Let $\mathcal{B}_\mathbb{R}$ denote the Borel σ-algebra on $\mathbb{R}$, i.e. the smallest σ-algebra in $\mathbb{R}$ generated by the open sets in $\mathbb{R}$. A* projection-valued measure *or PVM is a map $P : \mathcal{B}_\mathbb{R} \to B(\mathbf{H})$ satisfying the following properties:*

1. *For all $\Omega \in \mathcal{B}_\mathbb{R}$, $P(\Omega)^* = P(\Omega)$.*
2. *For all $\Omega \in \mathcal{B}_\mathbb{R}$, $P(\Omega)P(\Omega) = P(\Omega)$.*
3. *$P(\mathbb{R}) = \mathbf{1}$.*
4. *For all countable collections $\{\Omega\}_{i\in\mathbb{N}}$ of pairwise disjoint sets in $\mathcal{B}_\mathbb{R}$ and for all $\psi \in \mathbf{H}$,*

$$P\left(\bigcup_{i\in\mathbb{N}} \Omega_i\right)\psi = \sum_{i\in\mathbb{N}} P(\Omega_i)\psi.$$

Note that the properties 1. and 2. imply that each $P(\Omega)$ is an orthogonal projection operator, whereas 3. and 4. are reminiscent of the defining properties of a measure.[20]

One can make sense of integration with respect to a PVM P. That is to say, let $f : \mathbb{R} \to \mathbb{C}$ be measurable (with respect to $\mathcal{B}_\mathbb{R}$ and $\mathcal{B}_\mathbb{C}$), then it is possible to make sense of

$$\int_\mathbb{R} f\, dP$$

on an appropriate domain.

In particular, if f is simple, $f = \sum_{n=1}^N c_n \mathbf{1}_{\Omega_n}$, with $c_n \in \mathbb{C}$ and $\{\Omega_n\}$ pairwise disjoint sets in $\mathcal{B}_\mathbb{R}$, then

$$\int_\mathbb{R} f\, dP := \sum_{n=1}^N c_n P(\Omega_n)$$

is bounded operator on $\mathbf{H}$.

Definition 5.6. *For any PVM P and unit vector $\psi \in \mathbf{H}$, define a probability measure $\mu_\psi : \mathcal{B}_\mathbb{R} \to [0,1]$ as follows:*[21]

$$\mu_\psi(\Omega) = \langle \psi, P(\Omega)\psi \rangle.$$

We will see below that for measurable $f : \mathbb{R} \to \mathbb{C}$ and ψ in an appropriate subspace of $\mathbf{H}$:

$$\left\langle \psi, \left(\int_\mathbb{R} f\, dP \right) \psi \right\rangle = \int_\mathbb{R} f\, d\mu_\psi. \tag{5.1}$$

Exercise: Prove the above identity for simple f and $\psi \in \mathbf{H}$.

[20] Exercise: Show that $P(\emptyset) = 0$.

[21] Exercise: Show that μ_ψ^A is indeed a well-defined $\mathbb{R}$-valued probability measure on $\mathcal{B}_\mathbb{R}$.

Theorem 5.3 (Spectral Theorem)**.** *Let $A : \mathbf{H} \supseteq \mathcal{D}(A) \to \mathbf{H}$ be a self-adjoint operator. Then there is a unique projection-valued measure $P^A : \mathcal{B}_\mathbb{R} \to B(\mathbf{H})$, such that*

$$A = \int_\mathbb{R} \iota_\mathbb{R} \, dP^A,$$

with $\iota_\mathbb{R} : \mathbb{R} \to \mathbb{C}$ the inclusion map and $P^A(\Omega) = 0$ if $\Omega \subseteq \mathbb{R} \setminus \sigma(A)$, so the integral can be restricted to $\sigma(A)$.

In the literature, one sometimes encounters the alternative notations:

$$\int_\mathbb{R} \lambda \, P^A(d\lambda) \quad \text{and} \int_\mathbb{R} \lambda \, dP^A(\lambda).$$

We denote with μ_ψ^A the measure μ_ψ on $\mathcal{B}_\mathbb{R}$ associated to P^A.

Theorem 5.4 (Functional Calculus)**.** *Let $A : \mathbf{H} \supseteq \mathcal{D}(A) \to \mathbf{H}$ be a self-adjoint operator and let $f : \mathbb{R} \to \mathbb{C}$ be measurable. Then the following operator is well-defined*

$$f(A) := \int_\mathbb{R} f \, dP^A$$

on the dense subspace $\mathcal{D}(f(A)) = \{\psi \in \mathbf{H} \,|\, \int_\mathbb{R} |f|^2 \, d\mu_\psi^A\} \subseteq \mathbf{H}$. In particular, we can characterize $\mathcal{D}(A) = \{\psi \in \mathbf{H} \,|\, \int_\mathbb{R} |\lambda|^2 \, d\mu_\psi^A(\lambda)\}$.

Furthermore,

(i) *If $f : \mathbb{R} \to \mathbb{R}$, then $f(A)$ is self-adjoint.*

(ii) *If $f \in L^\infty(\mathbb{R}; \mathbb{C})$, then $f(A) \in B(\mathbf{H})$.*

(iii) *For all $\psi \in \mathcal{D}(f(A))$, $\langle \psi, f(A)\psi \rangle = \int_\mathbb{R} f d\mu_\psi^A$.*

Note that for all $m \in \mathbb{N}_0$ and ψ satisfying $\int_\mathbb{R} \lambda^{2m} \, d\mu_\psi^A(\lambda) < \infty$

$$\langle \psi, A^m \psi \rangle = \left\langle \psi, \left(\int_\mathbb{R} \lambda^m dP^A \right) \psi \right\rangle = \int_\mathbb{R} \lambda^m d\mu_\psi^A. \tag{5.2}$$

Exercise: Show that $\psi \in \mathcal{D}(A^k)$ for all $0 \leq k \leq m$. *Hint*: You may use that $f(A)g(A) = (fg)(A)$ and $\mathcal{D}(f(A)g(A)) = \mathcal{D}((fg)(A))$, for any $A : \mathcal{D}(A) \to \mathbf{H}$ self-adjoint and $f, g : \mathbb{R} \to \mathbb{C}$ measurable.

In the case of bounded operators, it can be shown that μ_ψ^A is the unique probability density satisfying (5.2).

5.2 Position and momentum operators

In this section, we define the position and momentum operators $\hat{x}^i$ and $\hat{p}_i$ with $1 \leq i \leq n$ on the Hilbert space $L^2(\mathbb{R}^n)$.

Proposition 5.5. *Let $V : \mathbb{R}^n \to \mathbb{R}$ be a measurable function. Let $\hat{V} : L^2(\mathbb{R}^n) \supseteq \mathcal{D}(\hat{V}) \to L^2(\mathbb{R}^n)$ be defined as follows:*

$$\begin{aligned} \mathcal{D}(\hat{V}) &= \{\psi \in L^2(\mathbb{R}^n) \,|\, V \cdot \psi \in L^2(\mathbb{R}^n)\}, \\ (\hat{V}\psi)(x) &= V(x)\psi(x). \end{aligned}$$

Then $\mathcal{D}(\hat{V})$ is dense in $L^2(\mathbb{R}^n)$ and $\hat{V}$ is a self-adjoint linear operator.

Proof. Let $E_m = \{x \in \mathbb{R}^n \,|\, |V(x)| \leq m\}$, so that $\cup_{m \in \mathbb{N}_0} E_m = \mathbb{R}^n$ and E_m are subsets of the Borel σ-algebra $\mathcal{B}_{\mathbb{R}^n}$. By construction, we have that for any $\psi \in L^2(\mathbb{R}^n)$, $\mathbf{1}_{E_m} \psi \in \mathcal{D}(\hat{V})$.

Hence, we can apply the Dominated Convergence Theorem to conclude that $\mathbf{1}_{E_m} \psi \to \psi$ with respect to the L^2 norm, so $\mathcal{D}(\hat{V})$ must be dense.

It is clear that $\hat{V}$ is symmetric with respect to the L^2-inner product. By Proposition 5.1(iv), $\hat{V}^*$ must therefore be an extension of $\hat{V}$. Now suppose that $\psi \in \mathcal{D}(\hat{V}^*)$, i.e.

$$\phi \mapsto \int_{\mathbb{R}^n} \overline{\psi(x)} V(x)\phi(x)\, dx$$

defines a bounded linear functional on $\mathcal{D}(\hat{V})$ and

$$\int_{\mathbb{R}^n} \overline{\psi(x)} V(x)\phi(x)\, dx = \int_{\mathbb{R}^n} \overline{(\hat{V}^*\psi)(x)}\phi(x)\, dx.$$

or equivalently,

$$\int_{\mathbb{R}^n} (\overline{\psi(x)} V(x) - \overline{(\hat{V}^*\psi)(x)})\phi(x)\, dx = 0.$$

Now take $\chi = (\psi V - \hat{V}^*\psi)$. Then by the above identity, $\langle \chi, \phi\rangle = 0$ for all $\phi \in \mathcal{D}(\hat{V})$ and by $\overline{\mathcal{D}(\hat{V})} = L^2(\mathbb{R}^n)$, $(\mathcal{D}(\hat{V}))^\perp = 0$, so $\chi = 0$ (as an element of $L^2(\mathbb{R}^n)$) , which in turn implies that $V\psi = \hat{V}^*\psi$ in $L^2(\mathbb{R}^n)$ and hence, $\psi \in \mathcal{D}(\hat{V})$. We infer that $\mathcal{D}(\hat{V}^*) \subseteq \mathcal{D}(\hat{V})$, from which $\mathcal{D}(\hat{V}^*) = \mathcal{D}(\hat{V})$ follows by the fact that $\hat{V}^*$ is an extension of $\hat{V}$. □

Corollary 5.6. *The position operators $\hat{x}^i$, with $1 \le i \le n$, are self-adjoint on the domains $\mathcal{D}(\hat{x}^i) = \{\psi \in L^2(\mathbb{R}^n) \,|\, x^i\psi \in L^2(\mathbb{R}^n)\}$.*

We interpret the position operator as a multiplication operator in Fourier space.

Proposition 5.7. (i) *For each $1 \le i \le n$, define $\hat{p}_i : L^2(\mathbb{R}^n) \supseteq \mathcal{D}(\hat{p}_i) \to L^2(\mathbb{R}^n_x)$ as follows: let $\mathcal{F} : L^2_x(\mathbb{R}^n) \to L^2_k(\mathbb{R}^n)$ denote the Fourier transform and let*

$$\mathcal{D}(\hat{p}_i) = \{\psi \in L^2(\mathbb{R}^n_x) \,|\, k_i\mathcal{F}(\psi) \in L^2(\mathbb{R}^n_k)\},$$
$$\hat{p}_i\psi = \mathcal{F}^{-1}(\hbar\hat{k}_i\mathcal{F}(\psi)).$$

Then $\hat{p}_i$ is self-adjoint.

(ii) *We can alternatively characterize:*

$$\mathcal{D}(\hat{p}_i) = \{\psi \in L^2(\mathbb{R}^n_x) \,|\, \partial_{x_i}\psi \in L^2(\mathbb{R}^n_x)\},$$
$$\hat{p}_i\psi = -i\hbar\partial_{x^i}\psi$$

with $\partial_{x^i}\psi$ denoting a distributional derivative.

Proof. "(i)": By Proposition 5.5, the multiplication operators $\hat{k}_i\psi := k_i\psi$ are self-adjoint on $\mathcal{F}(\mathcal{D}(\hat{p}_i))$. By the unitarity of $\mathcal{F}$, $\hat{p}_j = \hbar\mathcal{F}^{-1}\hat{k}_i\mathcal{F}$ must also be self-adjoint on $\mathcal{D}(\hat{p}_i)$.

"(ii)": We will only sketch the proof. It relies on the fact that for all $\chi \in C^\infty_c(\mathbb{R}^n)$, the distribution derivative $\partial_{x^j}\psi \in L^2(\mathbb{R}^n)$ of $\psi \in L^2(\mathbb{R}^n)$ satisfies by Plancherel's theorem:

$$\langle \mathcal{F}(\chi), \mathcal{F}(\partial_{x^j}\psi)\rangle = \langle \chi, \partial_{x^j}\psi\rangle = -\langle \partial_{x^j}\chi, \psi\rangle = -\langle i\hat{k}_j\mathcal{F}(\chi), \mathcal{F}(\psi)\rangle = \langle \mathcal{F}(\chi), i\hat{k}_j\mathcal{F}(\psi)\rangle.$$

Since χ was arbirary, it can be shown that $\mathcal{F}(\partial_{x^j}\psi)(k) = ik_j\mathcal{F}(\psi)(k)$ for almost every k. By the bijectivity of $\mathcal{F}$, it therefore holds that $\partial_{x^j}\psi = \mathcal{F}^{-1}(ik_j\mathcal{F}(\psi))$ almost everywhere. □

We will encounter moreover the Laplacian Δ, which by analogous arguments, can also shown to be self-adjoint on appropriate domains. We leave the proof as an Exercise.

Proposition 5.8. *Define $\Delta : L^2(\mathbb{R}^n) \supset \mathcal{D}(\Delta) \to L^2(\mathbb{R}^n)$ as follows:*

$$\mathcal{D}(\Delta) = \{\psi \in L^2(\mathbb{R}^n_x) \,|\, |k|^2\mathcal{F}(\psi) \in L^2(\mathbb{R}^n_k)\},$$
$$\Delta\psi = -\mathcal{F}^{-1}(|k|^2\mathcal{F}(\psi)).$$

Then Δ is self-adjoint. We have that $\mathcal{D}(\Delta) = W^{2,2}(\mathbb{R}^n) = H^2(\mathbb{R}^n)$ and $\Delta\psi$ as defined above agrees with $\Delta\psi$ defined in the distributional sense.

We can associate to a Hamiltonian

$$H(x,p) = \sum_{i=1}^{n} \frac{p_i^2}{2m} + V(x)$$

the operator

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + \hat{V}.$$

Operators of the form $\hat{H}$ are also called *Schrödinger operators.*

By the above properties,

$$\langle \psi, -\frac{\hbar^2}{2m}\Delta\psi\rangle = \langle \mathcal{F}^{-1}(\mathcal{F}(\psi)), \frac{\hbar^2}{2m}\mathcal{F}^{-1}(|k|^2\mathcal{F}(\psi))\rangle = \langle \mathcal{F}(\psi), \frac{\hbar^2}{2m}|k|^2\mathcal{F}(\psi)\rangle \geq 0.$$

One can show that $\hat{H}$ is self-adjoint under suitable assumptions on V.

Theorem 5.9. *Let $V : \mathbb{R}^n \to \mathbb{R}$ be a measurable function such that we can decompose $V = V_1 + V_2$, with $V_1 \in L^p(\mathbb{R}^n)$, where $p > \frac{n}{2}$ and $p \geq 2$, and with $V_2 \in L^\infty(\mathbb{R}^n)$. Then $\hat{H} : \mathcal{D}(\Delta) \to \mathbf{H}$ is self-adjoint and bounded below, i.e. there exists a $c \in \mathbb{R}$ such that*

$$\langle \psi, \hat{H}\psi\rangle \geq c|\psi|^2$$

for all $\psi \in \mathcal{D}(\Delta) = W^{2,2}(\mathbb{R}^n)$.

We will leave the proof of Theorem 5.9 for later.

Remark 5.3. *Theorem 5.9 illustrates an important difference between classical and quantum mechanics. Suppose V_1 is unbounded, e.g. $V_1(x) = -\frac{Q^2}{|x|}$ in the case of the Hamiltonian corresponding to an electron orbiting a hydrogen atom. Then in classical mechanics, the energy (kinetic+potential) can be made arbitrarily negative by considering as initial data $p = 0$ and x close to the origin. In contrast, the energy in quantum mechanics is bounded below by the* ground state energy

$$E_{GS} = \inf_{\psi \in W^{2,2}(\mathbb{R}^3)} \frac{\langle \psi, \hat{H}\psi\rangle}{\langle \psi, \psi\rangle} \geq c.$$

This lower bound property is called "stability of the first kind":

This difference is sometimes attributed to the fact that in quantum mechanics, one cannot localize both position and momentum, which is known as the uncertainty principle*. As we will later see, it is more accurate to say that the kinetic part of $\langle \psi, \hat{H}\psi\rangle$ controls the potential part via a Sobolev inequality, so the potential part cannot be much bigger than the kinetic part, in contrast to the situation in classical mechanics.*

Let $\psi \in \mathcal{D}(\hat{p}_j\hat{x}_i) \cap \mathcal{D}(\hat{x}_i\hat{p}_j)$ for all $1 \leq i, j \leq n$,

$$[\hat{x}^i, \hat{p}_j]\psi = i\hbar\delta^i_j\psi.$$

Suppose that instead of defining $\hat{x}_i$ and $\hat{p}_i$ as above, we started instead with two self-adjoint operators A, B satisfying

$$[A_i, B_j] = i\hbar\delta_{ij}\mathbf{1},$$

which are our candidates for position and momentum operators. We first decompose $\mathbf{H} = \bigoplus_l V_l$, with V_l the smallest closed subspaces that are invariant under all A_i and B_i.

Then it turns out that, under additional technical assumptions on A_i and B_i, on each V_l, there exists a unitary operator $U_l : V_l \to L^2(\mathbb{R}^n)$ such that $U_l A_i U_l^{-1} = \hat{x}_i$ and $U_l B_i U_L^{-1} = \hat{p}_i$. This is known as the Stone–von Neumann theorem. It may be interpreted as the statement that, up to conjugation with unitary operators, we may take $\mathbf{H} = L^2(\mathbb{R}^n)$ and represent the functions x_i and p_i by the operators $\hat{x}_i$ and $\hat{p}_i$.

5.3 The dynamic postulates of quantum mechanics

Recall that

$$[\hat{x}^i, \hat{p}_j] = i\hbar\delta^i_j.$$

This resembles very much the identity

$$\{x^i, p_j\} = \delta^i_j$$

where $\{\cdot,\cdot\} : C^\infty(\mathbb{R}^{2n}) \times C^\infty(\mathbb{R}^{2n}) \to C^\infty(\mathbb{R}^{2n})$ is the *Poisson bracket* which we saw in the earlier part of the course:

$$\{f, g\} = \sum_{j=1}^{n} \partial_{x^j} f \partial_{p_j} g - \partial_{p_j} f \partial_{x^j} g.$$

If $t \mapsto (x, p)(t)$ is a solution to Hamilton's equations of classical mechanics, then we also saw that

$$\frac{df}{dt}(x(t), p(t)) = \{f, H\}(x(t), p(t)).$$

If we want expectation values of observables to evolve in time like classical observables, the correspondence

$$\{\cdot,\cdot\} \longleftrightarrow \frac{1}{i\hbar}[\cdot,\cdot]$$

suggests

$$\frac{d\langle\hat{f}\rangle_\psi}{dt} = \frac{1}{i\hbar}\langle[\hat{f}, \hat{H}]\rangle_\psi.$$

Let $\hat{H}$ be as in Theorem 5.9. If we take the viewpoint that ψ is time dependent and the observables are time-dependent, this is guaranteed by the following postulate:

Postulate 4. *The time evolution of a respresentation of a physical state $\psi \in \mathcal{D}(\hat{H})$ is governed by the equation:*

$$\frac{d\psi}{dt} = \frac{1}{i\hbar}\hat{H}\psi. \tag{5.3}$$

The equation (5.11) is called the *Schrödinger equation.*

Indeed, from Postulate 4, (sesqui)linearity and self-adjointness of $\hat{H}$, it follows that for appropriate $\psi \in \mathbf{H}$

$$\frac{d\langle\hat{f}\rangle_\psi}{dt}(t) = \frac{d}{dt}\langle\psi(t), \hat{f}\psi(t)\rangle = \langle\frac{1}{i\hbar}\hat{H}\psi(t), \hat{f}\psi(t)\rangle + \langle\psi, \frac{1}{i\hbar}\hat{f}\hat{H}\psi(t)\rangle = \frac{1}{i\hbar}\langle\psi, [\hat{f}, \hat{H}]\psi(t)\rangle = \frac{1}{i\hbar}\langle[\hat{f}, \hat{H}]\rangle_\psi(t).$$

EXERCISE: Determine the conditions on the domain of ψ that guarantee that the above computation makes sense.

In particular, for $\hat{f} = \mathbf{1}$, this implies that

$$\frac{d}{dt}|\psi|^2(t) = \frac{1}{i\hbar}\langle[\mathbf{1}, \hat{H}]\rangle_\psi(t) = 0.$$

So if $\psi(0)$ is a unit vector, $\psi(t)$ will also be a unit vector. The time evolution is therefore norm preserving.

One can alternatively make the following postlulate

Postulate 4'. *The time evolution of observables $\hat{f} : \mathcal{D}(\mathbf{H}) \to \mathbf{H}$ is governed by the equation:*

$$\frac{d\hat{f}}{dt} = \frac{1}{i\hbar}[\hat{f}, \hat{H}]. \tag{5.4}$$

Postulate 4' also immediately implies that $\frac{d\langle\hat{f}\rangle_\psi}{dt} = \frac{1}{i\hbar}\langle[\hat{f}, \hat{H}]\rangle_\psi$. Postulate 4 is called the *Schrödinger picture* and Postulate 4' is called the *Heisenberg picture.*

We will show that the Schrödinger equation can be associated to *1-parameter unitary groups.*

Definition 5.7. *A* 1-parameter unitary group *is a family of unitary operators* $U(t) : \mathbf{H} \to \mathbf{H}$ *with* $t \in \mathbb{R}$ *such that*

- $U(0) = \mathbf{1}$,
- $U(s)U(t) = U(s+t)$ *for all* $s, t \in \mathbb{R}$.

A 1-parameter unitary group is strongly continuous *if moreover*

$$\lim_{t\to 0} |U(t)\psi - \psi| = 0$$

for all $\psi \in \mathbf{H}$.

We can associate to a strongly continuous 1-parameter unitary group a kind of "derivative" at $t = 0$:

Definition 5.8. *If* $U(\cdot)$ *is a strongly continuous 1-parameter unitary group on* $\mathbf{H}$*, then the* infinitesimal generator *of* $U(\cdot)$ *is the linear operator* $A : \mathbf{H} \supseteq \mathcal{D}(A) \to \mathbf{H}$*, with*

$$A\psi = \lim_{t\to 0} \frac{1}{i}\frac{U(t)\psi - \psi}{t},$$
$$\mathcal{D}(A) = \left\{ \psi \in \mathbf{H} \,|\, \lim_{t\to 0} \frac{1}{i}\frac{U(t)\psi - \psi}{t} \text{ exists} \right\}.$$

We will now see that

$$U(t) = e^{itA}$$

define a strongly continuous 1-parameter unitary group if A is self-adjoint. In the discussion of the Spectral Theorem, we saw that we can apply functions on $\mathbb{R}$ to self-adjoint operators as follows ("functional calculus"):

$$f(A) = \int_{\sigma(A)} f(\lambda)\, dP^A(\lambda)$$

to obtain an operator that is well-defined on the domain $\mathcal{D}(f(A)) = \{\psi \in \mathbf{H} \,|\, \int_{\mathbb{R}} |f|^2\, d\mu_\psi^A\} \subseteq \mathbf{H}$ for $f : \mathbb{R} \to \mathbb{R}$ a bounded measurable function. Furthermore, for $f, g : \mathbb{R} \to \mathbb{R}$ bounded and measurable, it is possible to show that $(fg)(A) = f(A)g(A)$.

Since $\mathbb{R} \ni \lambda \mapsto e^{it\lambda}$ is bounded for $t \in \mathbb{R}$, e^{itA} is well defined.

Proposition 5.10. *Suppose* $A : \mathbf{H} \supseteq \mathcal{D}(A) \to \mathbf{H}$ *is self-adjoint. Then* $U(t) = e^{itA}$ *defines a strongly continuous 1-parameter unitary group. Furthermore, for all* $\psi \in \mathbf{H}$*, the limit*

$$\lim_{t\to 0} \frac{1}{i}\frac{U(t)\psi - \psi}{t}$$

is well-defined if and only if $\psi \in \mathcal{D}(A)$ *and the limit is equal to* $A\psi$.

Proof. Denote $f_t(\lambda) = e^{it\lambda}$. Since $f_t(\lambda)\overline{f_t(\lambda)} = 1$, we have by the multiplicative property of the functional calculus that $f_t(A)f_t(A)^* = f_t(A)^* f_t(A) = \mathbf{1}$, so $f_t(A)$ is unitary (and bounded). It is therefore well-defined on the domain $\mathbf{H}$.

Since $f_0(A) = \mathbf{1}$ and $f_{t+s} = f_t f_s$, $U(t) = f_t(A)$ defines a 1-parameter unitary group. To establish strong continuity, note that

$$|U(t)\psi - \psi|^2 = \langle U(t)\psi - \psi, U(t)\psi - \psi\rangle = \langle (U^*(t) - \mathbf{1})(U(t) - \mathbf{1})\psi, \psi\rangle = \int_{\sigma(A)} |e^{it\lambda} - 1|^2\, d\mu_\psi^A(\lambda).$$

By the Dominated Convergence the integral on the RHS vanishes as $t \to 0$, so $U(\cdot)$ is strongly continuous.

Now, let $\psi \in \mathcal{D}(A)$. Then

$$\left| \frac{1}{i}\frac{U(t)\psi - \psi}{t} - A\psi \right| = \int_{\sigma(A)} \left| \frac{1}{i}\frac{e^{it\lambda} - 1}{t} - \lambda \right|^2 d\mu_\psi^A(\lambda). \tag{5.5}$$

We will show that RHS vanishes as $t \to 0$ by Dominated Convergence. First, note by the fundamental theorem of calculus that

$$\left|e^{it\lambda} - 1\right| = \left|\int_0^\lambda \frac{d}{d\lambda}(e^{it\lambda})\, d\lambda\right| \leq |t||\lambda|.$$

so

$$\left|\frac{1}{i}\frac{e^{it\lambda}-1}{t} - \lambda\right|^2 \leq \lambda^2.$$

Since

$$\int_{\sigma(A)} \lambda^2\, d\mu_\psi^A(\lambda) = \langle A\psi, A\psi\rangle < \infty$$

the function $\lambda \mapsto \lambda^2$ is integrable with respect to $d\mu_\psi^A(\lambda)$. This means that we can apply once again the Dominated Convergence Theorem to conclude that the RHS of (5.5) goes to zero as $t \to 0$.

Now suppose $\psi, \phi \in \mathcal{D}(B)$, with B the infinitesimal generator of $U(\cdot)$. Then

$$\begin{aligned}
\langle \phi, B\psi\rangle &= \lim_{t\to 0}\left\langle \phi, \frac{1}{i}\frac{U(t)\psi - \psi}{t}\right\rangle \\
&= \lim_{t\to 0}\left\langle -\frac{1}{i}\frac{U^*(t)\phi - \phi}{t}, \psi\right\rangle \\
&= \lim_{t\to 0}\left\langle \frac{1}{i}\frac{U(-t)\phi - \phi}{-t}, \psi\right\rangle \\
&= \langle B\phi, \psi\rangle.
\end{aligned}$$

Note that by the above $\mathcal{D}(A) \subseteq \mathcal{D}(B)$, so B is a symmetric operator and an extension of A.

Exercise:Symmetric operators B that are extensions of self-adjoint operators A must satisfy $\mathcal{D}(A) = \mathcal{D}(B)$ and $B = A$. □

Corollary 5.11. *Let $\hat{H} : L^2(\mathbb{R}^n) \supseteq \mathcal{D}(\hat{H}) \to L^2(\mathbb{R}^n)$ be a self-adjoint Hamiltonian operator. Then the initial value problem for the Schrödinger equation*

$$\begin{aligned}
\partial_t\psi(t,x) &= \frac{1}{i\hbar}(\hat{H}\psi)(t,x) \quad \text{in} \quad \mathbb{R}_t \times \mathbb{R}^n_x, \\
\psi(0,\cdot) &= \psi_0 \in \mathcal{D}(\hat{H})
\end{aligned}$$

admits a unique solution $\psi \in C^0([-T,T];\mathcal{D}(\hat{H})) \cap C^1([-T,T];L^2_x(\mathbb{R}^n))$ for any $T \in \mathbb{R}$, with $\psi(t,x) = e^{\frac{1}{i\hbar}t\hat{H}}\psi_0$.

Proof. By Proposition 5.10, $\psi(t,x) = U(t)\psi_0 = e^{-\frac{i}{\hbar}t\hat{H}}\psi_0$ is well-defined with infinitesimal generator $-\frac{1}{\hbar}\hat{H}$ and

$$\partial_t\psi(t,x) = \lim_{h\to 0}\frac{\psi(t+h,x)-\psi(t,x)}{t} = i\lim_{h\to 0}\frac{(U(h)U(t)\psi_0)(x) - (U(t)\psi_0)(x)}{it} = -\frac{i}{\hbar}(\hat{H}U(t)\psi_0)(x) = \frac{1}{i\hbar}(\hat{H}\psi)(t,x),$$

which is the Schrödinger equation.

By the strong continuity of $U(\cdot)$, we moreover have that the map $t \mapsto \psi(t,\cdot)$ is continuous. □

It turns out that every strongly continuous unitary group produces a self-adjoint operator.

Theorem 5.12 (Stone's theorem)**.** *The infinitesimal generator A of a strongly continuous unitary group $U(\cdot)$ is a unique, well-defined self-adjoint operator with $\mathcal{D}(A) \subseteq \mathbf{H}$ dense and $U(t) = e^{itA}$.*

By the above theorem, we could have also arrived at the Schrödinger equation by demanding that time evolution behaves according to a strongly continuous 1-parameter group. This would, however, not tell us that the self-adjoint infinitesimal generator should be the operator corresponding to the Hamiltonian of classical mechanics.

The final postulate is also known as the postulate of "wave function collapse".

Postulate 5. *Let f be an observable. Consider a physical system in a state represented by $\psi \in \mathcal{D}(\hat{f})$ and suppose that a measurement of $\hat{f}$ produces an outcome contained in $\sigma(\hat{f}) \supseteq \Omega \in \mathcal{B}_{\mathbb{R}}$. Then, immediately after the measurement the state will change ("collapse") to the state*

$$\psi_{\hat{f},\Omega} = \frac{P^{\hat{f}}(\Omega)\psi}{|P^{\hat{f}}(\Omega)\psi|},$$

with $P^{\hat{f}} : \mathcal{B}_{\mathbb{R}} \to B(\mathbf{H})$ the PVM associated to $\hat{f}$.[22]

By combining Postulates 3 and 5, we have that the new probability measure associated to $\hat{f}$ directly after a measurement whose value sits in Ω will be $\mu^{\hat{f}}_{\psi_{\hat{f},\Omega}}$.

In particular, if the point spectrum $\sigma_p(\hat{f}) \neq \emptyset$ and the measurement outcome is $\lambda \in \sigma_p(\hat{f})$, then $P^{\hat{f}}(\{\lambda\})$ will correspond to a projection to the eigenspace of λ and the associated probability measure will be a sum of Dirac measures.

In the case of the position operator, $\hat{x}$, which has a purely continuous spectrum (Exercise), we have that

$$(P^{\hat{x}}(\Omega)\psi)(x) = \mathbf{1}_{\Omega}(x)\psi(x).$$

The more precise the position measurement, the smaller the set Ω and the more the probability measure associated to $\psi_{\hat{x},\Omega}$ is localized.

The interpretation of Postulate 5 and its role in the time-evolution of the state is the source of a lot of ongoing debate, often of a philosophical nature.

5.4 The uncertainty principle

Definition 5.9. *Let $A : \mathbf{H} \supseteq \mathcal{D}(A) \to \mathbf{H}$ be a symmetric operator and let $\psi \in \mathcal{D}(A)$ with $|\psi| = 1$. Then we define the standard deviation $\Delta_\psi A$ as follows:*

$$\Delta_\psi A = \sqrt{\langle (A - \langle A \rangle_\psi \mathbf{1})^2 \rangle_\psi}.$$

We will also refer to A as the uncertainty *of A in a state represented by ψ.*

The goal of this section is to establish the following inequality, called the *Heisenberg uncertainty principle*:

$$\Delta_\psi \hat{x} \cdot \Delta_\psi \hat{p} \geq \frac{\hbar}{2},$$

for ψ with $|\psi| = 1$ in an appropriate subset of $\mathbf{H}$. This inequality tells us that if we choose ψ to be supported in a small interval so that $\Delta_\psi \hat{x}$ is very small, then $\Delta_\psi \hat{p}$ must necessarily be large, and similarly, the other way around: of we choose ψ so that $\Delta_\psi \hat{p}$ is very small, then $\Delta_\psi \hat{x}$ must be very large.

Another way of thinking about this is the following: suppose ψ is localized around a point $x_0 \in \mathbb{R}$, then the Fourier transform $\mathcal{F}(\psi)$ cannot also be localized around a point $p_0 \in \mathbb{R}$.

By Postulate 5, the uncertainty principle implies that we cannot simultanously measure position and momentum. Indeed, if we measure position (with small measurement error), then ψ will collapse to a state localized around the measurement value $x_0 \in \mathbb{R}$. If we then measure the momentum, it can no longer be localized around $x_0 \in \mathbb{R}$. It is fundamentally impossible to measure position and momentum precisely. The reason that this does not create issues on macroscopic scales is that $\hbar$ is *very* small in macroscopic units, i.e.

$$\hbar = 1.055 \times 10^{-34} J \cdot s.$$

To prove the uncertainty principle, we first introduce some notation for the domains of products of operators.

[22] Stated in this precise way, "wave function collapse" is also known as the *von Neumann–Lüders postulate.*

Definition 5.10. *Let A, B be linear operators on $\mathbf{H}$ with domains $\mathcal{D}(A)$ and $\mathcal{D}(A)$, respecetively. We define AB to be the operator with domain*

$$\mathcal{D}(AB) = \{\psi \in \mathcal{D}(B) \mid B\psi \in \mathcal{D}(A)\},$$

such that $AB\psi = A(B\psi)$.

Theorem 5.13. *Let A, B be symmetric operators and $\psi \in \mathcal{D}(AB) \cap \mathcal{D}(BA)$, such that $|\psi| = 1$. Then*

$$\Delta_\psi A \Delta_\psi B \geq \frac{1}{2} |\langle [A, B] \rangle_\psi|$$

Proof. Define $A' := A - \langle \psi, A\psi \rangle \mathbf{1}$ on $\mathcal{D}(A)$ and $B' := B - \langle \psi, B\psi \rangle \mathbf{1}$ on $\mathcal{D}(B)$. It can easily be shown that A' and B' are also symmetric.

Observe that $(\Delta_\psi A)^2 = \langle A'\psi, A'\psi \rangle$ and $(\Delta_\psi B)^2 = \langle B'\psi, B'\psi \rangle$.

Now, apply Cauchy–Schwarz to obtain:

$$\langle A'\psi, A'\psi \rangle \langle B'\psi, B'\psi \rangle \geq |\langle A'\psi, B'\psi \rangle|^2 \geq |\Im \langle A'\psi, B'\psi \rangle|^2 = \left| \frac{1}{2} \left(\langle A'\psi, B'\psi \rangle - \langle B'\psi, A'\psi \rangle \right) \right|^2$$

By symmetry of A' and B' and $\psi \in \mathcal{D}(A'B') \cap \mathcal{D}(B'A')$:

$$(\Delta_\psi A)^2 (\Delta_\psi B)^2 = \langle A'\psi, A'\psi \rangle \langle B'\psi, B'\psi \rangle \geq \frac{1}{4} |\langle \psi, [A', B']\psi \rangle|^2 = \frac{1}{4} |\langle \psi, [A, B]\psi \rangle|^2 . \qquad \square.$$

Corollary 5.14. *Let A, B be symmetric operators such that $[A, B] = i\hbar\mathbf{1}$ and $\psi \in \mathcal{D}(AB) \cap \mathcal{D}(BA)$, with $|\psi| = 1$. Then*

$$\Delta_\psi A \Delta_\psi B \geq \frac{\hbar}{2}.$$

In particular, for all $\psi \in L^2(\mathbb{R})$ such that $\psi \in \mathcal{D}(\hat{x}\hat{p}) \cap \mathcal{D}(\hat{p}\hat{x})$ and $|\psi| = 1$,

$$\Delta_\psi \hat{x} \Delta_\psi \hat{p} \geq \frac{\hbar}{2}.$$

If we are not careful with domain considerations, we can produce violations of the uncertainty principle.

Let $\mathbf{H} = L^2[-1, 1]$. Let $A\psi(x) = x\psi(x)$ be the analogue of the position operator $\hat{x}$. Since A is now bounded, we have that $\mathcal{D}(A) = L^2[-1, 1]$ and A is self-adjoint.

Let $B = -i\hbar \frac{d}{dx}$ be the analogue of the momentum operator $\hat{p}$. We will take $\mathcal{D}(B) = \{\psi \in C^1([-1, 1]) \mid \psi(-1) = \psi(1)\}$. It can be shown that $\mathcal{D}(B)$ is dense in $L^2[-1, 1]$. As in the case of the usual position and momentum operators, we have that for all $\psi \in \mathcal{D}(B)$

$$[A, B]\psi = i\hbar\psi.$$

Note that for $\phi, \psi \in \mathcal{D}(B)$, we can integrate by parts to obtain

$$\langle \phi, B\psi \rangle = -i\hbar \int_{-1}^{1} \overline{\phi(x)} \frac{d\psi}{dx}(x)\, dx = -i\hbar(\overline{\phi(1)}\psi(1) - \overline{\phi(-1)}\psi(-1)) + i\hbar \int_{-1}^{1} \overline{\frac{d\phi}{dx}(x)}\psi(x)\, dx = \langle B\phi, \psi \rangle,$$

where we applied the boundary conditions in the definition of $\mathcal{D}(B)$. Hence, B is symmetric. To conclude that B is essentially self-adjoint, we will apply the following lemma:

Lemma 5.15. *Let $B : \mathbf{H} \supseteq \mathcal{D}(B) \to \mathbf{H}$ be a densely defined symmetric operator with a countable orthonormal basis of eigenvectors. Then B is essentially self-adjoint.*

Proof. Essential self-adjointness will follow if we can show that the ranges $\operatorname{ran}(B - i\mathbf{1})$ and $\operatorname{ran}(B + i\mathbf{1})$ are dense subspaces of $\mathbf{H}$ (see the problem sheet). Let $\{e_j\}$ denote the orthonormal basis of eigenvectors of B. Then $(B \pm i\mathbf{1})e_j = (\lambda_j - i)e_j$. Since $\lambda_j \in \mathbb{R}$, $\operatorname{ran}(B \pm i\mathbf{1})$ contains any non-zero multiple of e_j for all j. Hence, it must be dense in $\mathbf{H}$. $\square$

Observe now that

$$\psi_j(x) = \frac{1}{\sqrt{2}} e^{i\pi j x}$$

define a orthonormal basis of eigenvectors for B, so B must be essentially self-adjoint. Denote with $\overline{B}$ its closure, which must be self-adjoint. Note now that

$$(\Delta_{\psi_j} \overline{B})^2 = \langle B\psi_j - \langle \psi_j, B\psi_j\rangle \psi, B\psi_j - \langle \psi_j, B\psi_j\rangle\rangle = \langle \lambda_j\psi_j - \lambda_j\psi_j, \lambda_j\psi_j - \lambda_j\psi_j\rangle = 0.$$

Since $\psi_j \in \mathcal{D}(A)$, $\Delta_{\psi_j} A$ is also well-defined, and therefore

$$\Delta_{\psi_j} A \Delta_{\psi_j} \overline{B} = 0.$$

Why is this not in contradiction with the uncertainty principle? It is because $A\psi_j \notin \mathcal{D}(B)$ as it does not satisfy the required boundary conditions. Hence $\psi \notin \mathcal{D}(AB)$, which is required for the uncertainty principle to hold.

In the case of the position and momentum operators on $L^2(\mathbb{R}^n)$, a stronger version of the uncertainty property holds, which we will state without proof.

Theorem 5.16. *Let $\hat{x}_j$ and $\hat{p}_j$ denote the position and momentum operators on $L^2(\mathbb{R}^n)$. If $\psi \in \mathcal{D}(\hat{x}_j) \cap \mathcal{D}(\hat{p}_j)$ and $|\psi| = 1$, then,*

$$\Delta_\psi \hat{x}_j \Delta_\psi \hat{p}_j \geq \frac{\hbar}{2}.$$

5.5 The self-adjointness of Schrödinger operators

We will now consider the following Hamiltonian or Schrödinger operators on $\mathbf{H} = L^2(\mathbb{R}^n)$:

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + \hat{V},$$

with measurable $\hat{V}$.

Since both $-\frac{\hbar^2}{2m}\Delta$ and $\hat{V}$ are self-adjoint on $\mathcal{D}(\Delta) \cap \mathcal{D}(\hat{V})$, you may think that establishing self-adjointness of the sum is straightforward. In particular, if $\hat{V}$ is very singular, (essential) self-adjointness may fail on natural domains.

Definition 5.11. *If A and B are unbounded operators on $\mathbf{H}$, then we take $A + B$ to be the operator with domain $A + B := \mathcal{D}(A) \cap \mathcal{D}(B)$ and $(A + B)\psi = A\psi + B\psi$.*

Theorem 5.17 (Kato–Rellich)**.** *Let A and B be self-adjoint linear operators on $\mathbf{H}$ with $\mathcal{D}(A) \subseteq \mathcal{D}(B)$. Suppose that there exist $a \in [0, 1)$, $b \in (0, \infty)$, such that for all $\psi \in \mathcal{D}(A)$*

$$|B\psi| \leq a|A\psi| + b|\psi|.$$

Then $A + B$ is self-adjoint on $\mathcal{D}(A)$. Furthermore, if $A \geq 0$, i.e. $\langle A\phi, \phi\rangle \geq 0$ for all $\phi \in \mathcal{D}(A)$, then

$$\sigma(A + B) \subseteq \left[-\frac{b}{1-a}, \infty\right).$$

Proof. Consider the operator $A + i\mu\mathbf{1}$, with $\mu \in \mathbb{R}_+$ to be determined. Then, for any $\psi \in \mathcal{D}(A)$,

$$(A + B + i\mu\mathbf{1})\psi = (B(A + i\mu\mathbf{1})^{-1} + \mathbf{1})(A + i\mu\mathbf{1})\psi, \tag{5.6}$$

where we used that $(A+i\mu\mathbf{1})^{-1}$ is a well-defined bounded linear operator (the resolvent) and $(A+i\mu\mathbf{1})^{-1}\phi \in \mathcal{D}(A)$ for all $\phi \in \mathbf{H}$, since $-i\mu \notin \sigma(A) \subseteq \mathbb{R}$. Now, note that

$$\begin{aligned}
|\psi|^2 &= |A(A + i\mu\mathbf{1})^{-1}\psi + i\mu(A + i\mu\mathbf{1})^{-1}\psi|^2 \\
&= |A(A + i\mu\mathbf{1})^{-1}\psi|^2 + \mu^2|(A + i\mu\mathbf{1})^{-1}\psi|^2 + \langle A(A + i\mu\mathbf{1})^{-1}\psi, i\mu(A + i\mu\mathbf{1})^{-1}\psi\rangle \\
&\quad + \langle i\mu(A + i\mu\mathbf{1})^{-1}\psi, A(A + i\mu\mathbf{1})^{-1}\psi\rangle.
\end{aligned}$$

By self-adjointness of A and sequilinearity of the inner product, the last two terms cancel, so

$$\mu^2|(A+i\mu\mathbf{1})^{-1}\psi|^2 + |A(A+i\mu\mathbf{1})^{-1}\psi|^2 = |\psi|^2,$$

from which it follows that $||(A+i\mu\mathbf{1})^{-1}|| \leq \frac{1}{\mu}$ and $||A(A+i\mu\mathbf{1})^{-1}|| \leq 1$.

By the invoking the inequality assumption on B, we therefore have that for all $\psi \in \mathbf{H}$

$$\begin{aligned}|B(A+i\mu\mathbf{1})^{-1}\psi| &\leq a|A(A+i\mu\mathbf{1})^{-1}\psi| + b|(A+i\mu\mathbf{1})^{-1}\psi| \\ &\leq \left(a + \frac{b}{\mu}\right)|\psi|.\end{aligned}$$

Now we take μ sufficiently large such that $a + \frac{b}{\mu} < 1$. Then for $C := B(A+i\mu\mathbf{1})^{-1}$, we have that $||C|| < 1$. It can then easily be shown that

$$(\mathbf{1}+C)^{-1} = \sum_{n\in\mathbb{N}_0} C^n$$

is a well-defined bounded linear operator, so $\mathrm{ran}(B(A+i\mu\mathbf{1})^{-1}+\mathbf{1}) = \mathbf{H}$. Together with the fact that that $\mathrm{ran}(A \pm i\mu\mathbf{1}) = \mathbf{H}$ iff A is self-adjoint (see problem sheet), it follows after applying (5.6) that $(A+B+i\mu\mathbf{1}) : \mathcal{D}(A) \to \mathbf{H}$ is surjective.

Repeating the above with μ replaced by $-\mu$ also tells use that $A+B-i\mu\mathbf{1} : \mathcal{D}(A) \to \mathbf{H}$ is surjective. Since $\mathrm{ran}(A+B\pm i\mu\mathbf{1}) = \mathbf{H}$, we must, by the above observation, therefore have that $A+B$ is self-adjoint.

Now suppose A is non-negative. Note that then $\sigma(A) \subseteq [0,\infty)$ (Exercise). We will consider $A+\lambda\mathbf{1}$, with $\lambda \in [0,\infty)$. We proceed as above with $i\mu$ replaced by λ to obtain:

$$\begin{aligned}|\psi|^2 = |A(A+\lambda\mathbf{1})^{-1}\psi|^2 + \lambda^2|(A+\lambda\mathbf{1})^{-1}\psi|^2 + \langle A(A+\lambda\mathbf{1})^{-1}\psi, \lambda(A+\lambda\mathbf{1})^{-1}\psi\rangle \\ + \langle \lambda(A+\lambda\mathbf{1})^{-1}\psi, A(A+\lambda\mathbf{1})^{-1}\psi\rangle, \quad (5.7)\end{aligned}$$

where we note that $(A+\lambda\mathbf{1})^{-1}$ is a well-defined bounded linear operator with $(A+\lambda\mathbf{1})^{-1}\phi \in \mathcal{D}(A)$ for all $\phi \in \mathbf{H}$, since $-\lambda \notin \sigma(A) \subseteq [0,\infty)$.

By the fact that $\langle A\phi,\phi\rangle \geq 0$, we moreover have that the last two terms on the RHS of (5.7) are non-negative, so that

$$|\psi|^2 \geq |A(A+\lambda\mathbf{1})^{-1}\psi|^2 + \lambda^2|(A+\lambda\mathbf{1})^{-1}\psi|^2.$$

Hence, $|(A+\lambda\mathbf{1})^{-1}\psi| \leq \frac{1}{\lambda}$. Proceeding as above with λ replacing $i\mu$, we obtain

$$|B(A+\lambda\mathbf{1})^{-1}\psi| \leq \left(a + \frac{b}{\lambda}\right)|\psi|$$

We have that $a + \frac{b}{\lambda} < 1$ if and only if $\lambda > \frac{b}{1-a}$. Repeating the above argument gives us moreover that $\mathrm{ran}(A+B+\lambda\mathbf{1}) = \mathbf{H}$. Since for any self-adjoint operator C, $\mathrm{ran}(C)^\perp = \ker C^*$ (problem sheet), we can use self-adjointness of $A+B+\lambda\mathbf{1}$ to conclude that $\ker(A+B+\lambda\mathbf{1}) = \ker(A+B+\lambda\mathbf{1})^* = \mathrm{ran}(A+B+\lambda\mathbf{1})^\perp = \{0\}$.

This implies that $A+B+\lambda\mathbf{1}$ is invertible with bounded inverse, since $||(A+\lambda\mathbf{1})^{-1}|| < \frac{1}{\lambda}$), so $-\lambda \notin \sigma(A+B)$ and $\sigma(A+B) \subseteq [-\frac{b}{1-a},\infty)$. □

To be able to satisfy the inequality assumption in the Kato–Rellich Theorem, we need the following important inequalities on L^p-norms, which we will state without proof:

Lemma 5.18. (i) *(Hölder inequality) Let $p,q \in [1,\infty]$ and $r \in [1,\infty)$, with $\frac{1}{p}+\frac{1}{q} = \frac{1}{r}$ and let $f \in L^p(\mathbb{R}^n)$, $g \in L^q(\mathbb{R}^n)$. Then $fg \in L^r(\mathbb{R}^n)$, with*

$$||fg||_{L^r(\mathbb{R}^n)} = ||f||_{L^q(\mathbb{R}^n)}||g||_{L^p(\mathbb{R}^n)}.$$

(ii) *(Hausdorff–Young inequality) Let $p \in [1,2]$ and $q \in [2,\infty)$, such that $\frac{1}{q}+\frac{1}{p} = 1$. Then the Fourier transform is well-defined as the map $\mathcal{F} : L^p(\mathbb{R}^n) \to L^q(\mathbb{R}^n)$ and*

$$||\mathcal{F}(f)||_{L^q(\mathbb{R}^n)} \leq ||f||_{L^p(\mathbb{R}^n)}.$$

Recall the statement of Theorem 5.9:

Theorem. *Let $V : \mathbb{R}^n \to \mathbb{R}$ be a measurable function such that we can decompose $V = V_1 + V_2$, with $V_1 \in L^p(\mathbb{R}^n)$, where $p > \frac{n}{2}$ and $p \geq 2$, and with $V_2 \in L^\infty(\mathbb{R}^n)$. Then $\hat{H} : \mathcal{D}(\Delta) \to L^2(\mathbb{R}^n)$ is self-adjoint and bounded below, i.e. there exists a constant $c \in \mathbb{R}$ such that*

$$\langle \psi, \hat{H}\psi \rangle \geq c|\psi|^2$$

for all $\psi \in \mathcal{D}(\Delta) = W^{2,2}(\mathbb{R}^n)$.

We are now in a position to prove this theorem.

Proof of Theorem 5.9. We will take $A = -\frac{\hbar^2}{2m}\Delta$ and $B = \hat{V}$ and apply the Kato–Rellich Theorem. First, we need to show that $\mathcal{D}(\hat{V}) \subseteq \mathcal{D}(\Delta) = \{\psi \in L^2(\mathbb{R}^n_x) \,|\, |k|^2\mathcal{F}(\psi) \in L^2(\mathbb{R}^n_k)\}$.

Observe first that that there exists a constant $c_{n,p} > 0$ such that for $t \in \mathbb{R}_+$

$$\int_{\mathbb{R}^n} (1 + t|k|^2)^{-p}\, dk = \int_0^\infty \int_{\mathbb{S}^{n-1}} (1 + t|k|^2)^{-p}|k|^{n-1}\, d|k| d\sigma_{\mathbb{S}^{n-1}} < c_{n,p}^p t^{-\frac{n}{2}}$$

if $-2p + n - 1 < -1$ or $p > \frac{n}{2}$, in which case $(1 + t|k|^2)^{-1} \in L^p(\mathbb{R}^n)$ and $||(1 + t|k|^2)^{-1}||_{L^p(\mathbb{R}^n)} < c_{n,p}t^{-\frac{n}{2p}}$. By Hölder's inequality,

$$\begin{aligned} ||\mathcal{F}(\psi)||_{L^r(\mathbb{R}^n)} &= ||(1 + t|k|^2)^{-1}(1 + t|k|^2)\mathcal{F}(\psi)||_{L^r(\mathbb{R}^n)} \\ &\leq ||(1 + t|k|^2)^{-1}||_{L^p(\mathbb{R}^n)}||(1 + t|k|^2)\mathcal{F}(\psi)||_{L^2(\mathbb{R}^n)} \\ &\leq c_{n,p}t^{1-\frac{n}{2p}}(t^{-1}||\psi||_{L^2(\mathbb{R}^n)} + ||\Delta\psi||_{L^2(\mathbb{R}^n)}) \end{aligned}$$

for $\frac{1}{r} = \frac{1}{p} + \frac{1}{2}$.

By the Hausdorff–Young inequality (applied to $\mathcal{F}(\psi)$) we then obtain

$$||\psi||_{L^q(\mathbb{R}^n)} \leq ||\mathcal{F}(\psi)||_{L^r(\mathbb{R}^n)} \leq c_{n,p}t^{1-\frac{n}{2p}}(t^{-1}||\psi||_{L^2(\mathbb{R}^n)} + ||\Delta\psi||_{L^2(\mathbb{R}^n)})$$

for $\frac{1}{q} + \frac{1}{r} = 1$, if $1 \leq r \leq 2$, which requires $p \geq 2$.

Now, using that $\frac{1}{q} + \frac{1}{p} = \frac{1}{q} + \frac{1}{r} - \frac{1}{2} = \frac{1}{2}$, we can apply Hölder again to the product $V_1\psi$ to conclude that $V_1\psi \in L^2(\mathbb{R}^n)$ if $\psi \in \mathcal{D}(\Delta)$ and, since V_2 is bounded, we immediately have that $V_2\psi \in L^2(\mathbb{R}^n)$, so $\psi \in \mathcal{D}(\hat{V})$.

We now turn to the inequality assumed in Kato–Rellich. The same Hölder inequality as above gives

$$\begin{aligned} ||V\psi||_{L^2(\mathbb{R}^n)} &\leq ||V_1||_{L^p(\mathbb{R}^n)}||\psi||_{L^q(\mathbb{R}^n)} + ||V_2||_{L^\infty(\mathbb{R}^n)}||\psi||_{L^2(\mathbb{R}^n)} \\ &\leq c_{n,p}||V_1||_{L^p(\mathbb{R}^n)}t^{1-\frac{n}{2p}}(||\Delta\psi||_{L^2(\mathbb{R}^n)} + t^{-1}||\psi||_{L^2(\mathbb{R}^n)}) + ||V_2||_{L^\infty(\mathbb{R}^n)}||\psi||_{L^2(\mathbb{R}^n)}. \end{aligned}$$

Since $2p > n$, we can take t sufficiently small such that $a := \frac{2m}{\hbar^2}c_{n,p}||V_1||_{L^p(\mathbb{R}^n)}t^{1-\frac{n}{2p}} < 1$ so that the assumption in Kato–Rellich is satisfied with $A = -\frac{\hbar^2}{2m}\Delta$ and $B = \hat{V}$.

Note that smaller t results in a larger constant b in the lower bound in Kato–Rellich. □

The above theorem can be improved to include potentials which do not satisfy the assumptions in the theorem but are non-negative, i.e. $V \geq 0$. This includes for example, the harmonic oscillator potential $V(x) = x^2$. We state the corresponding theorem without proof.

Theorem 5.19. *Let $V : \mathbb{R}^n \to \mathbb{R}$ be a measurable function such that we can decompose $V = V_1 + V_2 + V_+$, with $V_1 \in L^p(\mathbb{R}^n)$, where $p = 2$ (if $n \leq 3$), $p > 2$ (if $n = 4$) and $p = \frac{n}{2}$ if ($n \geq 5$), $V_2 \in L^\infty(\mathbb{R}^n)$, and with $V_+ \in L^2_{\text{loc}}(\mathbb{R}^n)$ and $V_+ \geq 0$.[23] Then $\hat{H} : \mathcal{D}(\Delta) \to L^2(\mathbb{R}^n)$ is self-adjoint and bounded below, i.e. there exists a $c \in \mathbb{R}$ such that*

$$\langle \psi, \hat{H}\psi \rangle \geq c|\psi|^2$$

for all $\psi \in \mathcal{D}(\Delta) = W^{2,2}(\mathbb{R}^n)$.

[23] The space $L^2_{\text{loc}}(\mathbb{R}^n)$ consists of measurable functions f such that $\chi_K f \in L^2(\mathbb{R}^n)$ for all compact $K \subset \mathbb{R}^n$.

5.6 The free Schrödinger equation

We consider now the Schrödinger equation corresponding to the Schrödinger operator $\hat{H} = -\frac{\hbar^2}{2m}\Delta$:

$$\begin{aligned} \partial_t \psi &= \frac{i\hbar}{2m}\Delta\psi, \\ \psi(0,\cdot) &= \psi_0. \end{aligned} \tag{5.8}$$

We will analyse solutions to this equations by means of the Fourier transform in x. Note the transformation of $-i\partial_{x^i}$ to multiplication k_i under the Fourier transform, when acting on suitably regular functions.

In Fourier space, the Schrödinger equation therefore becomes

$$\partial_t \mathcal{F}(\psi) = -\frac{i\hbar|k|^2}{2m}\mathcal{F}(\psi).$$

This equation can easily be solved:

$$\mathcal{F}(\psi)(t,k) = \mathcal{F}(\psi_0)(k)e^{-\frac{i\hbar|k|^2}{2m}t}.$$

The above expression suggests that $\psi(t,x)$ can therefore be obtained via an inverse Fourier transform:

$$\psi(t,x) = \frac{1}{(2\pi)^{\frac{n}{2}}}\int_{\mathbb{R}^n} \mathcal{F}(\psi_0)(k)e^{i\left(k\cdot x - \frac{\hbar|k|^2}{2m}t\right)}\,dk.$$

In the proposition below, we show that the above expression indeed solves the initial value problem (5.8). For this, we observe that the exponential in the integrand solves the free Schrödinger equation:

$$\left(\partial_t - \frac{i\hbar}{2m}\Delta\right)e^{i\left(k\cdot x - \frac{\hbar|k|^2}{2m}t\right)} = 0.$$

Theorem 5.20. *Let $\psi_0 \in L^2(\mathbb{R}^n)$. Then the corresponding solution to (5.8) (in a distributional sense) is given by:*

$$\psi(t,\cdot) = \mathcal{F}^{-1}\left(\mathcal{F}(\psi_0)(k)e^{i\left(k\cdot x - \frac{\hbar|k|^2}{2m}t\right)}\right) \tag{5.9}$$

In particular, if ψ_0 is a Schwartz function, then

$$\psi(t,x) = \frac{1}{(2\pi)^{\frac{n}{2}}}\int_{\mathbb{R}^n} \mathcal{F}(\psi_0)(k)e^{i\left(k\cdot x - \frac{\hbar|k|^2}{2m}t\right)}\,dk.$$

Proof. Suppose that ψ_0 is a Schwartz function. Note first that

$$\frac{\psi(t+h,x)-\psi(t,x)}{h} = \frac{1}{(2\pi)^{\frac{n}{2}}}\int_{\mathbb{R}^n} \mathcal{F}(\psi_0)(k)e^{ik\cdot x}\frac{e^{-i\frac{\hbar|k|^2}{2m}(t+h)} - e^{-i\frac{\hbar|k|^2}{2m}t}}{h}\,dk$$

Note that, by the mean-value theorem

$$\left|\frac{e^{-i\frac{\hbar|k|^2}{2m}(t+h)} - e^{-i\frac{\hbar|k|^2}{2m}t}}{h}\right| \leq \frac{\hbar}{2m}|k|^2.$$

Since $\mathcal{F}$ maps Schwartz functions to Schwartz functions, $\mathcal{F}(\psi_0)$ is Schwartz and $|k|^2|\mathcal{F}(\psi_0)|$ is integrable and we can apply the Dominated Convergence Theorem to conclude that:

$$\partial_t\psi(t,x) = \frac{1}{(2\pi)^{\frac{n}{2}}}\int_{\mathbb{R}^n} \mathcal{F}(\psi_0)(k)\partial_t e^{i\left(k\cdot x - \frac{\hbar|k|^2}{2m}t\right)}\,dk$$

Similarly, using that for $h \in \mathbb{R}^n$ with $h^j = a\delta_r^j$

$$\left| \frac{e^{ik\cdot(x+h)} - e^{ik\cdot x}}{a} \right| \leq |k_r|.$$

We have that

$$\partial_{x^r}\psi(t,x) = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} \mathcal{F}(\psi_0)(k) \partial_{x^r} e^{i\left(k\cdot x - \frac{\hbar|k|^2}{2m}t\right)}\, dk$$

and repeating this, we obtain

$$\partial_t\psi(t,x) - \frac{i\hbar}{2m}\Delta\psi(t,x) = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} \mathcal{F}(\psi_0)(k) \left(\partial_t - \frac{i\hbar}{2m}\Delta\right) e^{i\left(k\cdot x - \frac{\hbar|k|^2}{2m}t\right)}\, dk = 0.$$

Furthermore,

$$\mathcal{F}(\psi)(t,k) = \mathcal{F}(\psi_0)(k) e^{-\frac{i\hbar|k|^2}{2m}t}.$$

Now let $\psi_0 \in L^2(\mathbb{R}^n)$ and, by density of Schwartz functions in $L^2(\mathbb{R}^n)$, let $\psi_0^{(j)}$ be a sequence of Schwartz functions approaching ψ_0. Denote with $\psi^{(j)}$ the corresponding solutions to (5.8). Then

$$\psi^{(j)}(t,\cdot) := \mathcal{F}^{-1}(\mathcal{F}(\psi_0^{(j)}) e^{-\frac{i\hbar|k|^2}{2m}t})$$

are well–defined Schwartz functions. Since, $\mathcal{F}$ is well-defined and unitary on $L^2(\mathbb{R}^n)$, $\{\psi^{(j)}(t,\cdot\}$ form a Cauchy sequence in $L^2(\mathbb{R}^n)$ and admit a limit $\psi(t,\cdot)$ which satisfies $\mathcal{F}(\psi(t,\cdot)) = \mathcal{F}(\psi_0)e^{-\frac{i\hbar|k|^2}{2m}t}$.

It remains to show that for all $\chi \in C_c^\infty(\mathbb{R}_t \times \mathbb{R}_x^n)$

$$\int_{\mathbb{R}\times\mathbb{R}^n} \overline{\psi} \left(\partial_t\chi - \frac{i\hbar}{2m}\Delta\chi\right) dxdt = 0.$$

Exercise: Show that the above is equivalent to $(\partial_t - \frac{i\hbar}{2m}\Delta)\psi = 0$ if $\psi \in C^2(\mathbb{R}_t \times \mathbb{R}_x^n)$.

By Plancherel and integrating by parts in t:

$$\begin{aligned}
\int_{\mathbb{R}\times\mathbb{R}^n} \overline{\psi} \left(\partial_t\chi - \frac{i\hbar}{2m}\Delta\chi\right) dxdt &= \int_{\mathbb{R}\times\mathbb{R}^n} \overline{\mathcal{F}(\psi)(t,k)} \left(\partial_t\mathcal{F}(\chi) + \frac{i\hbar}{2m}|k|^2\mathcal{F}(\chi)\right) dkdt \\
&= \int_{\mathbb{R}\times\mathbb{R}^n} \overline{\mathcal{F}(\psi_0)(k)} e^{\frac{i\hbar|k|^2}{2m}t} \left(\partial_t\mathcal{F}(\chi) + \frac{i\hbar}{2m}|k|^2\mathcal{F}(\chi)\right) dkdt \\
&\overset{\text{int. by pt.}}{=} \int_{\mathbb{R}\times\mathbb{R}^n} \overline{\mathcal{F}(\psi_0)(k)} e^{\frac{i\hbar|k|^2}{2m}t} \left(-\frac{i\hbar|k|^2}{2m}\mathcal{F}(\chi) + \frac{i\hbar}{2m}|k|^2\mathcal{F}(\chi)\right) dkdt = 0.
\end{aligned}$$

□

In the proposition below, we will see that we can think of solutions ψ to (5.8) as convolution with $K_t : \mathbb{R}^n \to \mathbb{C}$, which is defined as follows:

$$K_t(x) := (2\pi)^{-n} \int_{\mathbb{R}^n} e^{ik\cdot x} e^{-i\frac{\hbar|k|^2 t}{2m}}\, dk = \left(\frac{m}{2\pi i\hbar t}\right)^{\frac{n}{2}} e^{\frac{im|x|^2}{2\hbar t}}.$$

For this, we need the following lemma.

Lemma 5.21. *Let $\psi, \phi \in L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$. Then $\phi * \psi \in L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$ and*

$$(2\pi)^{-\frac{n}{2}}\mathcal{F}(\phi * \psi) = \mathcal{F}(\phi)\mathcal{F}(\psi).$$

Proof. We can write

$$\begin{aligned}\mathcal{F}(\phi * \psi)(k) &= (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n_x} \left(\int_{\mathbb{R}^n_y} \phi(x-y)\psi(y)\, dy \right) e^{-ik\cdot x}\, dx \\ &= (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n_x} \left(\int_{\mathbb{R}^n_y} e^{-ik\cdot(x-y)}\phi(x-y)e^{-ik\cdot y}\psi(y)\, dy \right) dx \\ &\overset{\text{Fubini}}{=} (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n_z \times \mathbb{R}^n_y} e^{-ik\cdot z}\phi(z)e^{-ik\cdot y}\psi(y)\, dydz \\ &= (2\pi)^{\frac{n}{2}} \mathcal{F}(\phi)\mathcal{F}(\psi). \end{aligned}$$

□

Theorem 5.22. *Suppose $\psi_0 \in L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$. Then ψ as defined in (5.9) can be expressed as follows for all $t \neq 0$:*

$$\psi(t,\cdot) = K_t * \psi_0,$$

or

$$\psi(t,x) = \left(\frac{m}{2\pi i\hbar t}\right)^{\frac{n}{2}} \int_{\mathbb{R}^n} e^{\frac{im|x-y|^2}{2\hbar t}} \psi_0(y)\, dy.$$

Proof. Consider $B_j(0)$ the ball of radius j around $0 \in \mathbb{R}^n$. Then $1_{B_j(0)}K_t \in L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$. By Lemma 5.21, we have that

$$\mathcal{F}(1_{B_j(0)}K_t * \psi_0) = (2\pi)^{\frac{n}{2}} \mathcal{F}(1_{B_j(0)}K_t)\mathcal{F}(\psi_0). \tag{5.10}$$

We would like to conclude that

$$(2\pi)^{\frac{n}{2}} \mathcal{F}(1_{B_j(0)}K_t)\mathcal{F}(\psi_0) \xrightarrow{L^2} e^{-i\frac{\hbar|k|^2 t}{2m}} \mathcal{F}(\psi_0)$$

with respect to the L^2 norm as $j \to \infty$. Since $\psi_0 \in L^2(\mathbb{R}^n)$ and one can show that 1) the above convergence holds pointwise (see definition of K_t) and 2) $\mathcal{F}(1_{B_j(0)}K_t)$ can be bounded uniformly by a constant (Exercise: prove 1) and 2)), we can apply the Dominated Convergence Theorem to conclude the above L^2-convergence.

Now, by Plancherel, and the identity (5.10), we must also have L^2-convergence of the corresponding inverse Fourier transforms:

$$(1_{B_j(0)}K_t) * \psi_0 \xrightarrow{L^2} \mathcal{F}^{-1}(e^{-i\frac{\hbar|k|^2 t}{2m}} \mathcal{F}(\psi_0))$$

As clearly, the left-hand side above also converges pointwise $K_t * \psi_0$ in $L^2(\mathbb{R}^n)$, since $\psi_0 \in L^1(\mathbb{R}^n)$, and the pointwise limit must coincide with the L^2 limit, we can conclude that:

$$K_t * \psi_0 = \mathcal{F}^{-1}(e^{-i\frac{\hbar|k|^2 t}{2m}} \mathcal{F}(\psi_0)) \in L^2(\mathbb{R}^n).$$

Note that the right-hand side above is equal to ψ as defined in (5.9). □

Remark 5.4. *By the conservation of $||\psi(t,\cdot)||_{L^2(\mathbb{R}^n)}$ in t and the fact that we can estimate*

$$||\psi(t,\cdot)||_{L^\infty(\mathbb{R}^n)} \leq \left(\frac{|m|}{2\pi\hbar}\right)^{\frac{n}{2}} ||\psi_0||_{L^1(\mathbb{R}^n)} t^{-\frac{n}{2}},$$

we can see that ψ disperses *or spreads out as $t \to \infty$.*

Remark 5.5. *Note that the free Schrödinger equation satisfies the* infinite speed of propagation property*. Indeed, consider initial data ψ_0 with support in $B_R(0)$ for some $R > 0$. Let $x \in \mathbb{R}^n$, with $|x|$ arbitrarily large. Then*

$$\psi(t,x) = \left(\frac{m}{2\pi i\hbar t}\right)^{\frac{n}{2}} \int_{B_R(0)} e^{\frac{im(x-y)^2}{2\hbar t}} \psi_0(y)\, dy$$

will not be vanishing for general data ψ_0. This means that arbitrarily far away points in space are instantaneously affected by initially localized perturbations.

5.7 Multiple particles and mixed states

In quantum mechanics, N distinguishable particles[24] in $\mathbb{R}^3$ are represented by a state $\psi \in L^2(\mathbb{R}^{3N})$. We can make sense of statements about the position $x_j^{(k)}$ and momentum $p_j^{(k)}$ coordinates of the k-th particle by considering appropriate operators $\hat{x}_j^{(k)}$ and $\hat{p}_j^{(k)}$, $j = 1, 2, 3$, which only involve the coordinates (x_j, p_j) on the k-th copy of $\mathbb{R}^3$ in $\mathbb{R}^{3N}$.

Suppose we would like to associate to the k-th particle a unit vector $\psi^{(k)} \in L^2(\mathbb{R}^3)$. Then we encounter an ambiguity as there is no unique way of decomposing a vector $\psi \in L^2(\mathbb{R}^{3N})$ into N-vectors in $L^2(\mathbb{R}^3)$. The notation of a state as introduced in Postulate 1 is therefore inadequate to describe a *subsystem* within a physical system.

Since there is no issue with associating quantum observables to classical observables that are restricted to the phase space describing a subset of particles, there is also no issue with describing the corresponding expectation values. Indeed, consider the Hilbert space $L^2(\mathbb{R}^6)$. The components x_j, $j = 1, 2, 3$, of the position vector $x \in \mathbb{R}^6$ describe the position of particle 1. The corresponding expectation value is then given by:

$$\langle \hat{x}_j \rangle = \langle \psi, \hat{x}_j \psi \rangle.$$

We will therefore try to redefine a "state" by *starting* from a family of expectation values. We start by considering expectation values associated to bounded linear operators.

Definition 5.12. *A linear map $\Phi : B(\mathbf{H}) \to \mathbb{C}$ is a* family of expectation values *if the following conditions hold:*

1. $\Phi(\mathbf{1}) = 1$,
2. $\Phi(A) \in \mathbb{R}$ *if A is self-adjoint,*
3. $\Phi(A) \geq 0$ *if A is self-adjoint and $A \geq 0$,*
4. *Let $\{A_n\}$ be a strongly converging sequence in $B(\mathbf{H})$, i.e. there exists a $A \in B(\mathbf{H})$ such that for all $\psi \in \mathbf{H}$, $|A_n\psi - A\psi| \to 0$ as $n \to \infty$, then $\Phi(A_n) \to \Phi(A)$ in $B(\mathbf{H})$.*

We will see below that families of expectation values are closely linked to so-called *density matrices*.

Definition 5.13. *A* trace $\operatorname{tr} A$ *of an operator $A \in B(\mathbf{H})$ with $A \geq 0$ is defined as follows: let $\{e_j\}$ be an orthonormal basis of $\mathbf{H}$*[25]*, then*

$$\operatorname{tr} A = \sum_{j=1}^{\infty} \langle e_j, A e_j \rangle.$$

The operator $A \in B(\mathbf{H})$ is said to be trace class *if $\operatorname{tr} \sqrt{AA^*} < \infty$.*[26]

An operator $\rho \in B(\mathbf{H})$ is a density matrix if ρ is self-adjoint, $\rho \geq 0$ and $\operatorname{tr} \rho = 1$.

It can be shown (see Chapter VI of Reed–Simon Volume 1) that $\operatorname{tr}(AB) = \operatorname{tr}(BA) < \infty$ for A a trace class operator and $B \in B(\mathbf{H})$. Furthermore, it can be shown that self-adjoint trace class operators are compact, which implies that they admit a basis of eigenvectors.

We will state the following theorem without proof:

Theorem 5.23. *Let $\rho \in B(\mathbf{H})$ be a density matrix. Then the linear map $\Phi_\rho : B(\mathbf{H}) \to \mathbb{C}$,*

$$\Phi_\rho(A) = \operatorname{tr}(\rho A) = \operatorname{tr}(A\rho)$$

is a family of expectation values. Conversely, for any family of expectation values $\Phi : B(\mathbf{H}) \to \mathbb{C}$, there exists a unique density matrix ρ such that $\Phi = \Phi_\rho$.

[24] If the particle k and l are indistinguishable, then the classical observables should be invariant under $\mathbf{x}_k \in \mathbb{R}^3$ and $\mathbf{x}_l \in \mathbb{R}^3$.

[25] Exercise: Show that the trace is independent of the choice of orthonormal basis.

[26] Here $\sqrt{AA^*} = f(AA^*)$, with $f(z) = \sqrt{z}$, is defined via functional calculus applied to AA^*, using that AA^* is self-adjoint.

Recall the physics notation $|\psi\rangle\langle\psi|$ for the orthogonal projection onto the span of a unit vector ψ, i.e. $|\psi\rangle\langle\psi|(\phi) = \langle\psi, \phi\rangle\psi$. The proposition below demonstrates that via this operator, we can include our previous notion of a state.

Proposition 5.24. *For any unit vector $\psi \in \mathbf{H}$, $\rho = |\psi\rangle\langle\psi|$ is a density matrix and for any $A \in B(\mathbf{H})$:*

$$\operatorname{tr}(|\psi\rangle\langle\psi| A) = \langle\psi, A\psi\rangle = \langle A\rangle_\psi.$$

Proof. Since $|\psi\rangle\langle\psi|$ is an orthogonal projection, it is bounded, self-adjoint and non-negative. We compute its trace by considering a countable orthonormal basis $\{e_j\}$ of $\mathbf{H}$ with $e_1 = \psi$. Note that $\rho(e_j) = \delta_{1j} e_1$, so

$$\operatorname{tr}\rho = \sum_{j=1}^{\infty} \langle e_j, \rho e_j\rangle = \sum_{j=1}^{\infty} \delta_{1j}\langle e_j, e_1\rangle = 1.$$

Hence, $\rho = |\psi\rangle\langle\psi|$ is a density matrix.

For any $A \in B(\mathbf{H})$, we moreover have that

$$\operatorname{tr}(|\psi\rangle\langle\psi| A) = \sum_{j=1}^{\infty} \langle e_j, \psi\rangle\langle\psi, Ae_j\rangle = \langle\psi, A\psi\rangle.$$

□

Note moreover that for $c \in \mathbb{C}$, with $|c| = 1$, $|c\psi\rangle\langle c\psi| = |\psi\rangle\langle\psi|$, so each element in the equivalence class $[\psi]$ (see Postulate 1) gives the same density matrix.

Definition 5.14. *A density matrix $\rho \in B(\mathbf{H})$ is a* pure state *if there exists a unit vector $\psi \in \mathbf{H}$ such that $\rho = |\psi\rangle\langle\psi|$. A density matrix $\rho \in B(\mathbf{H})$ is a* mixed state *if there exists no such unit vector $\psi \in \mathbf{H}$.*

We can identify (up to unitary maps) $L^2(\mathbb{R}^{3N})$ with the completion of $L^2(\mathbb{R}^3)\underbrace{\otimes \ldots \otimes}_{N} L^2(\mathbb{R}^3)$. We denote the completion of the tensor product of two Hilbert spaces $\mathbf{H}_1$ and $\mathbf{H}_2$ by $\mathbf{H}_1 \widehat{\otimes} \mathbf{H}_2$.

Proposition 5.25. *There exists a unique unitary map $U : L^2(\mathbb{R}^n)\widehat{\otimes}L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^{2n})$, such that for all $\psi, \phi \in L^2(\mathbb{R}^n)$*

$$U(\psi \otimes \phi)(x, y) = \psi(x)\phi(y).$$

Proof. Sketch of proof: Part 1: the existence and uniqueness of U restricted to $L^2(\mathbb{R}^n) \otimes L^2(\mathbb{R}^n)$ satisfying the desired property follows from the universal property of tensor products which says that to any bilinear map $B : L^2(\mathbb{R}^n) \times L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^{2n})$ corresponds a unique linear map U such that $U : L^2(\mathbb{R}^n) \otimes L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^{2n})$ with $U(\psi \otimes \phi) = B(\psi, \phi)$.

Note that $|U(\psi \otimes \phi)| = |\psi| \cdot |\phi|$. Since any element of $L^2(\mathbb{R}^n) \otimes L^2(\mathbb{R}^n)$ can be written as a linear combination of a finite number of elements of the form $\psi_j \otimes \phi_j$, we can conclude that U is an isometry. It therefore admits a unique isometric extension to the completion $L^2(\mathbb{R}^n)\widehat{\otimes}L^2(\mathbb{R}^n)$.

Part 2: To conclude unitarity of U, it remains to show surjectivity, i.e. $\operatorname{ran} U = L^2(\mathbb{R}^n)$. This is done by showing that $(\operatorname{ran} U)^\perp = \{0\}$. We will not prove this part.

□

We now consider a more general version of Postulate 1, adapted to the notion of mixed states and to the tensor product property above:

Postulate 1'. *A* state of a physical system *is a density matrix $\rho \in B(\mathbf{H})$, with $(\mathbf{H}, \langle\ ,\ \rangle)$ a Hilbert space. The state of a physical system composed of two subsystems associated to the Hilbert spaces $\mathbf{H}_1$ and $\mathbf{H}_2$ is described by a density matrix $\rho \in B(\mathbf{H}_1 \widehat{\otimes} \mathbf{H}_2)$.*

If a pure state $\psi \in \mathbf{H}_1 \widehat{\otimes} \mathbf{H}_2$ is of the form $\psi_1 \otimes \psi_2$, with $\psi_1 \in \mathbf{H}_1$ and $\psi_1 \in \mathbf{H}_2$, we says ψ is *non-entangled*. Otherwise, we says ψ is *entangled*.

In the case of a single particle with spin s, $s = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$ moving in $\mathbb{R}^3$, the Hilbert space is given by $\mathbf{H} = L^2(\mathbb{R}^3)\hat{\otimes}V_s$ with V_s a complex vector space of dimension $2s+1$. We can identify $L^2(\mathbb{R}^3)\hat{\otimes}V_s \cong L^2(\mathbb{R}^3; V_s)$.

Now suppose we consider 2 identical particles of spin s. In view of the above theorem, a natural guess for the corresponding Hilbert space would be $L^2(\mathbb{R}^3; V_s)\hat{\otimes}L^2(\mathbb{R}^3; V_s) \cong L^2(\mathbb{R}^6; V_s \otimes V_s)$. However, in view of the *Spin-statistics theorem*, which goes beyond the scope of quantum mechanics, the following holds:

- In the case of spin $s = l \in \mathbb{N}_0$ we say the particles are *bosons* and we have to consider $L^2(\mathbb{R}^6; \mathrm{Sym}(V_s \otimes V_s))$, with $\mathrm{Sym}(V_s \otimes V_s)$ the symmetric $(2,0)$-tensors on V_s. More generally for N identical bosons, the relevant Hilbert space is $L^2(\mathbb{R}^{3N}; \mathrm{Sym}(\overbrace{V_s \otimes \ldots \otimes V_s}^{N}))$.
- In the case of $s = l + \frac{1}{2}$, $l \in \mathbb{N}_0$, we say the particles are *fermions* and we have to consider $L^2(\mathbb{R}^6; \mathrm{Alt}(V_s \otimes V_s))$, with $\mathrm{Alt}(V_s \otimes V_s)$ the antisymmetric $(2,0)$-tensors on V_s. In the case of N identical fermions, the relevant Hilbert space is $L^2(\mathbb{R}^{3N}; \mathrm{Alt}(\overbrace{V_s \otimes \ldots \otimes V_s}^{N}))$.

Since $\mathrm{tr}(\rho A)$ is only defined for $A \in B(\mathbf{H})$, we have to be a little careful with the interpretation of $\mathrm{tr}(\rho A)$ as an expectation value, in the case of unbounded A.

We keep Postulate 2 as is. We change Postulate 3 as follows:

Postulate 3'. *Consider an observable $\hat{f}$ corresponding to a function $f : \mathbb{R}^{2n} \to \mathbb{R}$. For a physical system in a state $\rho \in B(\mathbf{H})$, the result of the measurement of f is governed by a* probability measure $\mu_\rho^{\hat{f}} : \mathcal{B}_\mathbb{R} \to [0,1]$ *that is defined as follows:*

$$\mu_\rho^{\hat{f}}(\Omega) = \mathrm{tr}(\rho P^{\hat{f}}(\Omega)),$$

with $P^{\hat{f}} : \mathcal{B}_\mathbb{R} \to B(\mathbf{H})$ the PVM associated to $\hat{f}$ via the spectral theorem.

Note that in view of Postulate 3', the expectation value associated to the probability measure is given by:

$$\langle \hat{f} \rangle_\rho = \int_\mathbb{R} \lambda \, d\mu_\rho^{\hat{f}}(\lambda).$$

In the case of $A \in B(\mathbf{H})$, it holds that[27]

$$\mathrm{tr}(\rho A) = \int_\mathbb{R} \lambda \, d\,\mathrm{tr}(\rho P^A)(\lambda) = \int_\mathbb{R} \lambda \, d\mu_\rho^A(\lambda) = \langle A \rangle_\rho,$$

so the $B(\mathbf{H}) \ni A \mapsto \langle A \rangle_\rho$ satisfies the defining properties of an family of expectation values.

Recall that our original aim was to define states of N particles in such a way that we can uniquely split off the state corresponding to a single particle. With Postulate 1' and 3' this can be done by the proposition below. Given $A \in B(\mathbf{H}_1)$ and $C \in B(\mathbf{H}_2)$, we first denote with $A \otimes C \in B(\mathbf{H}_1 \widehat{\otimes} \mathbf{H}_2)$ the unique linear operator with

$$(A \otimes C)(\phi \otimes \psi) = A(\phi) \otimes C(\phi).$$

for all $\phi \in \mathbf{H}_1$ and $\psi \in \mathbf{H}_2$.

Proposition 5.26. *Let ρ be a density matrix on $\mathbf{H}_1 \widehat{\otimes} \mathbf{H}_2$. Then there exists a unique density matrix $\rho^{(1)}$ on $\mathbf{H}_1$ such that for all $A \in B(\mathbf{H}_1)$:*

$$\mathrm{tr}(\rho(A \otimes \mathbf{1})) = \mathrm{tr}(\rho^{(1)} A).$$

Proof. By Theorem 5.23, $\Phi = \mathrm{tr}(\rho((\cdot) \otimes \mathbf{1}))$ defines a family of expectation values on $B(\mathbf{H}_1)$, so there must exist a unique $\rho^{(1)}$ such that $\Phi = \Phi_{\rho^{(1)}}$. □

[27] For unbounded A, we could try to *define*:

$$\mathrm{tr}(\rho A) := \int_\mathbb{R} \lambda \, d\mu_\rho^{\hat{f}}(\lambda),$$

provided the integral is appropriately convergent. We will omit a careful analysis of this.

Hence, to each state $\rho \in B(\mathbf{H}_1 \widehat{\otimes} \mathbf{H}_2)$ of a composite system, there exists a unique state $\rho^{(1)} \in B(\mathbf{H}_1)$ that describes the subsystem corresponding to $\mathbf{H}_1$ and its associated probability measure satisfies for self-adjoint A on $\mathbf{H}_1$: for all $\Omega \in \mathcal{B}_{\mathbb{R}}$

$$\mu^A_{\rho^{(1)}}(\Omega) = \mathrm{tr}(\rho^{(1)} P^A(\Omega)) = \mathrm{tr}(\rho P^A(\Omega) \otimes \mathbf{1}) = \mu^{A \otimes \mathbf{1}}_{\rho}(\Omega),$$

so it produces the correct expectation value for operators restricted to $\mathbf{H}_1$.

Time-evolution takes the following form (ignoring issues of domain):

Postulate 4'. *The time evolution of a physical system in a state $\rho \in B(\mathbf{H})$ is governed by the equation:*

$$\frac{d\rho}{dt} = -\frac{1}{i\hbar}[\rho, \hat{H}] \tag{5.11}$$

and $\rho(t) = e^{-\frac{it}{\hbar}\hat{H}} \rho(0) e^{+\frac{it}{\hbar}\hat{H}}$.

Note the similarity of the above equation to the Liouville equation:

$$(\partial_t \rho)(t, \cdot) = -\{\rho(t, \cdot), H\}.$$

from Hamiltonian mechanics, which plays an important role in statistical mechanics as it represents a probability density. Note also that the probability of encountering particle 1 in an N-particle system at the 1-particle phase space point (x^1, p_1) is governed by the following probability density:

$$\rho^{(1)}(x^1, p_1) = \int_{\mathbb{R}^{6(N-1)}} \rho(x^1, p_1, x^2, p_2, \ldots, x^N, p_N) dx^2 dp^2 \ldots dx^N dp^N.$$

The above naturally leads us to an analogous, statistical interpretation of density matrices and mixed states. Suppose we prepare a (1-particle) system to lie in a state represented by $\psi \in \mathbf{H}$, $|\psi| = 1$, but there is a degree of uncertainty regarding exactly what state the system is in. Then we can describe the system by a density matrix, which encodes the probabilities that the system is in a set of different states. In other words, density matrices describe the state of a *statistical ensemble* of particles.

For example, let $\psi, \phi \in \mathbf{H}$ such that $|\psi| = |\phi| = 1$ and $\langle \psi, \phi \rangle = 0$, then

$$\rho = \frac{1}{3}|\psi\rangle\langle\psi| + \frac{2}{3}|\phi\rangle\langle\phi|$$

is a density matrix that can be interpreted as stating that the system is in state ψ with probability $\frac{1}{3}$ and in state ϕ with probability $\frac{2}{3}$.

Note that the notion of probability coming from the uncertainty about which state a system is in is fundamentally different from the notion of probability regarding measurement outcomes that is intrinsic to quantum mechanics and is present even if we know exactly what state a system is in.

Postulate 5'. *Let $\hat{f}$ be an observable corresponding to a function $f : \mathbb{R}^{2n} \to \mathbb{R}$. Consider a physical system in a state $\rho \in B(\mathbf{H})$. Suppose that a measurement of f produces an outcome contained in $\Omega \in \mathcal{B}_{\mathbb{R}}$, where $\Omega \subset \sigma(\hat{f})$. Then, immediately after the measurement, the state will change ("collapse") to the state*

$$\rho_{\hat{f},\Omega} = \frac{P^{\hat{f}}(\Omega) \rho P^{\hat{f}}(\Omega)}{Z},$$

with $Z := \mathrm{tr}(P^{\hat{f}}(\Omega) \rho P^{\hat{f}}(\Omega))$ and $P^{\hat{f}} : \mathcal{B}_{\mathbb{R}} \to B(\mathbf{H})$ the PVM associated to $\hat{f}$ via the spectral theorem.

Note that $P^{\hat{f}}(\Omega) \rho P^{\hat{f}}(\Omega)$ defines a positive operator with finite trace.

EXERCISE: Check that in the case $\rho = |\psi\rangle\langle\psi|$, Postulates 3'–5' imply Postulates 3–5, respectively.

In the proposition below, we establish several different ways of checking whether a state is pure.

Proposition 5.27. (i) *A density matrix $\rho \in B(\mathbf{H})$ corresponds to a pure state if and only if $\rho^2 = \rho$.*

(ii) *A density matrix $\rho \in B(\mathbf{H})$ corresponds to a pure state if and only if* $\operatorname{tr}\rho^2 = 1$.

(iii) *A density matrix $\rho \in B(\mathbf{H})$ corresponds to a pure state if and only if* $S(\rho) = \operatorname{tr}(-\rho\log\rho) = 0$. *The quantity $S(\rho)$ is called the* von Neumann entropy.

Proof. Suppose $\rho = |\psi\rangle\langle\psi|$, let $\{e_j\}$ be an orthonormal basis with $e_1 = \psi$. Then $\rho(e_j) = \delta_{1j}e_1$. Let $\phi \in \mathbf{H}$. Then we can write $\phi = \sum_{j=1}^{\infty}\phi^j e_j$, so

$$\rho^2(\phi) = \sum_{j=1}^{\infty}\phi^j\rho^2(e_j) = \phi^1 e_1 = \rho(\phi).$$

Hence $\rho^2 = \rho$.

This immediately implies that $\operatorname{tr}\rho^2 = \operatorname{tr}\rho = 1$ and $2\log\rho = \log\rho^2 = \log\rho$, so $\log\rho = 0$ and $S(\rho) = 0$.

Now suppose ρ is a density matrix. Since ρ is self-adjoint and compact, it has an orthonormal basis of eigenvectors $\{e_j\}$ with corresponding eigenvalues λ_j such that $\lambda_j \to 0$ as $j \to \infty$. Suppose that $\rho^2 = \rho$. We can then express:

$$\sum_{j\in\mathbb{N}_1}|\lambda_j|^2 = ||\rho||^2 = ||\rho^2||^2 = \sum_{j\in\mathbb{N}_1}|\lambda_j|^4.$$

This implies that

$$\sum_{j\in\mathbb{N}_1}|\lambda_j|^2(1-|\lambda_j|^2) = 0,$$

so $\lambda_j = 1$ or $\lambda_j = 0$. Since $1 = \operatorname{tr}\rho = \sum_{j\in\mathbb{N}_1}\lambda_j$, there exists precisely one j such that $\lambda_j = 1$. Hence, $\rho = |e_j\rangle\langle e_j|$.

Now suppose $\operatorname{tr}\rho^2 = 1$. Then $\operatorname{tr}\rho^2 = \operatorname{tr}\rho$, so

$$\sum_{j=1}^{\infty}\lambda_j^2 = \sum_{j=1}^{\infty}\lambda_j.$$

Using that $\lambda_j \geq 0$, as $\rho \geq 0$, this implies that

$$\sum_{j=1}^{\infty}\lambda_j(1-\lambda_j) = 0,$$

so, as above, there exists precisely one j such that $\lambda_j = 1$ and $\rho = |e_j\rangle\langle e_j|$.

Finally, suppose that $\operatorname{tr}(-\rho\log\rho) = 0$. Then

$$0 = \sum_{j=1}^{\infty}-\lambda_j\log\lambda_j.$$

Since all $\rho \geq 0$ and $\operatorname{tr}\rho = 1$, $0 \leq \lambda_j \leq 1$, so $-\lambda_j\log\lambda_j \geq 0$. By the vanishing of the above infinite sum, we must therefore have that $-\lambda_j\log\lambda_j = 0$ for all j, so either $\lambda_j = 1$ or $\lambda_j = 0$. By $\operatorname{tr}\rho = 1$, there is precisely one j such that $\lambda_j = 1$ and $\rho = |e_j\rangle\langle e_j|$. □

Since we can express $S(\rho) = \sum_{j\in\mathbb{N}_1}-\lambda_j\log\lambda_j$, with $0 \leq \lambda_j \leq 1$ the eigenvalues of ρ and $\sum_{j\in\mathbb{N}_1}\lambda_j = 1$, we see a strong resemblance to the Gibbs entropy from statistical mechanics: consider a classical system described by a discrete set of possible microstates, then the Gibbs entropy is given by

$$S_{\text{Gibbs}} = -k_B\sum_{j\in\mathbb{N}_1}p_j\log p_j,$$

with p_j the probability of the system being in the j-th microstate.

A Geometry

A.1 Geodesics and normal coordinates

Let $(\mathcal{M}, g)$ be a Riemannian or Lorentzian manifold and denote with ∇ the corresponding Levi–Civita connection.

We first look closer at the locality property of the covariant derivative.

Lemma A.1. *Let $p \in \mathcal{M}$ and $X, Y \in \Gamma(TM)$. Let U be an arbitrarily small neighbourhood containing p. Then $\nabla_X Y(p)$ depends only on $Y|_U$ and $X(p)$.*

Proof. Let $\phi \in C^\infty(\mathcal{M})$ be a smooth bump function such that $\operatorname{supp}\varphi \subset U$ and $\varphi(p) = 1$. Let $Y, \tilde{Y} \in \Gamma(T\mathcal{M})$ such that $Y|_U = \tilde{Y}|_U$. Denote $Z = Y - \tilde{Y}$. By linearity of ∇_X, it is sufficient to show that $\nabla_X Z(p) = 0$. Since Z vanishes on U, we have that $\varphi Z \equiv 0$. Hence, by the product rule for covariant derivatives:

$$0 = \nabla_X(\varphi Z)(p) = X(\varphi)(p)Z(p) + \varphi(p)\nabla_X Z(p) = 0 + 1 \cdot \nabla_X Z(p).$$

Now let $X, \tilde{X} \in \Gamma(T\mathcal{M}))$ be such that $X(p) = \tilde{X}(p)$ and define $V = X - \tilde{X}$. We then need to show that for any $Y \in \Gamma(T\mathcal{M}))$, $\nabla_V Y(p) = 0$. Let $p \in \mathcal{U}$, with $\mathcal{U}$ the domain of a coordinate chart $\{x^\mu\}$. Then we can express $V = V^\mu \partial_\mu$. Furthermore, we can write:

$$\nabla_V Y(p) = V^\mu(p)\nabla_{\partial_\mu} Y(p) = 0.$$

□

We will introduce the notion of the covariant derivative along curves corresponding to ∇. Let $\gamma : I \to \mathcal{M}$ be a smooth curve with $I \subset \mathbb{R}$ open. Then we define $\mathcal{T}(\gamma)$, the set of *vector fields along* $\gamma : I \to \mathcal{M}$, as follows:

$$\mathcal{T}(\gamma) = \{X : I \to T\mathcal{M} \,|\, X(t) \in T_{\gamma(t)}\mathcal{M} \,\forall t \in I\}.$$

Proposition A.2. *For each smooth curve $\gamma : I \to \mathcal{M}$, with $I \subset \mathbb{R}$ an open interval, ∇ determines a unique operator $D_t : \mathcal{T}(\gamma) \to \mathcal{T}(\gamma)$ satisfying the following properties:*

(i) *(Linearity) Let $X, Y \in \mathcal{T}(\gamma)$ and $\lambda \in \mathbb{R}$, then*

$$D_t(\lambda X + Y) = \lambda D_t X + D_t Y.$$

(ii) *(Product rule) Let $f \in C^\infty(I)$ and $X \in \mathcal{T}(\gamma)$. Then*

$$D_t(fX) = \dot{f}X + f D_t X.$$

(iii) *(Extensions) If $X \in \mathcal{T}(\gamma)$ is extendible to $\Gamma(T\mathcal{M})$, then for any extension $\widetilde{X} \in \Gamma(T\mathcal{M})$ of X,*

$$D_t X(t) = \nabla_{\dot{\gamma}(t)} \widetilde{X},$$

where $\nabla_{\dot{\gamma}(t)}$ is well-defined by Lemma A.1.

We refer to $D_t X$ as the covariant derivative of X along γ.

Proof. We first establish uniqueness. Let $t_0 \in I$. By Lemma A.1 and property (iii), $D_t X$ depends only on $X|_{(t_0-\epsilon, t_0+\epsilon)}$, with $\epsilon > 0$ arbitrarily small. Let $t_0 \subset U$, with U covered by a single coordinate chart $\{x^\mu\}$. We write $X(t) = X^\mu(t)\partial_\mu$. Since ∂_μ is extendible, we use all three properties of D_t to obtain:

$$\begin{aligned} D_t X(t_0) &= \dot{X}^\mu(t_0)\partial_\mu + X^\mu(t_0)\nabla_{\dot{\gamma}(t_0)}\partial_\mu \\ &= (\dot{X}^\nu(t_0) + \dot{X}^\mu(t_0)\dot{\gamma}(t_0)^\rho \Gamma^\nu_{\mu\rho}(\gamma(t_0))\partial_\nu. \end{aligned}$$

Hence, D_t must be unique if it exists. In fact, we can use the above expression to define D_t if $\gamma(I)$ lies in the domain of a single chart. If not, we can use it to define D_t locally and then conclude that the expressions agree when two charts overlap. □

Definition A.1. *We define the* acceleration *of curve $\gamma : \mathbb{R} \subseteq I \to \mathcal{M}$ as $D_t\dot{\gamma}$. We say γ is an affinely parametrized* geodesic *if $D_t\dot{\gamma} \equiv 0$, which we refer to as the geodesic equation.*

Proposition A.3. *Let $p \in \mathcal{M}$ and $X_p \in T_p\mathcal{M}$. Then there exists an open interval $0 \in I \subset \mathbb{R}$ and a smooth geodesic $\gamma : I \to \mathcal{M}$ such that*

$$\gamma(t_0) = p,$$
$$\dot{\gamma}(t_0) = X_p.$$

Any two such geodesics agree on their common domain.

Proof. The equation $D_t\dot{\gamma} \equiv 0$ reduces to a second-order ODE in the domain of a chart around p. Apply existence and uniqueness for ODE (Picard–Lindelöf). □

Let $X_p \in T_p\mathcal{M}$. Then we denote with γ_{X_p} the corresponding geodesic with $\gamma_{X_p}(0) = p$ and $\dot{\gamma}_{X_p}(0) = X_p$.

Proposition A.4. *Let $\gamma : I \to \mathcal{M}$ be a geodesic. Then*

$$\frac{d}{dt} g_{\gamma(t)}(\dot{\gamma}(t), \dot{\gamma}(t)) = 0.$$

Proof.

$$\frac{d}{dt} g_{\gamma(t)}(\dot{\gamma}(t), \dot{\gamma}(t)) = \nabla_{\dot{\gamma}} g(\dot{\gamma}, \dot{\gamma})(t) = 2g(D_t\dot{\gamma}, \dot{\gamma})(t) = 0.$$

□

Let g be a Lorentzian metric. We say $X \in T_p\mathcal{M}$ is *spacelike* if $g_p(X, X) > 0$, *timelike* if $g_p(X, X) < 0$ and *null* if $g_p(X, X) = 0$. By the above proposition, the corresponding geodesics γ_X can similarly be classified as timelike, spacelike or null geodesics.

We similarly say a general curve $\gamma : I \to \mathcal{M}$ is spacelike, timelike or null if the tangent vector field $\dot{\gamma}$ satisfies $g(\dot{\gamma}, \dot{\gamma}) > 0$, $g(\dot{\gamma}, \dot{\gamma}) < 0$ and $g(\dot{\gamma}, \dot{\gamma}) = 0$ respectively.

Remark A.1. *Recall that we already saw that for submanifolds on $\mathbb{R}^n$ with the metric induces by the Euclidean metric on $\mathbb{R}^n$ the geodesic equation corresponds to the Euler–Lagrange equations of the action:*

$$\mathcal{S}(\gamma) = \int_I g_{\gamma(t)}(\dot{\gamma}(t), \dot{\gamma}(t)\, dt.$$

This is also true when we restrict to spacelike or timelike curves in Lorentzian manifolds. However, all null curves satisfy $g_{\gamma(t)}(\dot{\gamma}(t), \dot{\gamma}(t)) = 0$ for all t, but they need not be geodesics.

Geodesics allow use to define a natural coordinate chart in the neighbourhood of any point in $\mathcal{M}$ called *normal coordinates*. We first define an exponential map.

Definition A.2. *Let $p \in \mathcal{M}$ and $\mathcal{E}_p := \{X \in T_p\mathcal{M} \,|\, \gamma_X : I \to \mathcal{M}$ well-defined with $[0, 1] \subset I\}$. Then the (restricted)* exponential map $\mathrm{Exp}_p : \mathcal{E}_p \to \mathcal{M}$ *is defined as:*

$$\mathrm{Exp}_p(X) = \gamma_X(1).$$

We use the notation "Exp" so as not to confuse this map with the exponential map "exp" on Lie groups.

Lemma A.5. *The exponential map Exp_p satisfies the following properties:*

(i) *For any $X \in T_pM$, $\gamma_{cX} = \gamma_X(ct)$, with $c \geq 0$, $t \in \mathbb{R}$ such that either side is well-defined.*

(ii) *For each $X \in \mathcal{E}_p$ we can express $\gamma_X(t) = \mathrm{Exp}_p(tX)$ for all t such that either side is well-defined.*

(iii) *$\mathcal{E}_p$ is starshaped with respect to 0, i.e. if $X \in \mathcal{E}_p$ then $tX \in \mathcal{E}_p$ for all $t \in [0, 1]$. Furthermore, there exists a $r > 0$ such that $B_r(0) \subset \mathcal{E}_p$.*

(iv) *The map Exp_p is smooth.*

Proof. We will first prove (i). Without loss of generality, we will show that if $\gamma_X(ct)$ is well-defined, then $\gamma_{cX}(t)$ is also well-defined. Indeed, if we instead start with the assumption that $\gamma_{cX}(t)$ is well-defined, we repeat the argument with X replaced with cX and c replaced with $\frac{1}{c}$.

Suppose the domain of $\gamma = \gamma_X$ is I, with $0 \in I \subset \mathbb{R}$ open. Define $\tilde{\gamma} : c^{-1}I \to \mathcal{M}$ by $\tilde{\gamma}(t) = \gamma(ct)$. Then $\tilde{\gamma}(0) = p$ and

$$\dot{\tilde{\gamma}}(0) = c\dot{\gamma}(0) = cX.$$

It remains to show that $\tilde{\gamma}$ is a geodesic. Let $\widetilde{D}_t$ and D_t be the covariant derivatives along γ and $\tilde{\gamma}$, respectively. We compute in coordinates:

$$\begin{aligned}\tilde{D}_t\dot{\tilde{\gamma}}^\nu(t) &= \ddot{\tilde{\gamma}}^\nu(t) + \dot{\tilde{\gamma}}^\mu(t)\dot{\tilde{\gamma}}^\rho(t)\Gamma^\nu_{\mu\rho}(\tilde{\gamma}(t)) \\ &= c^2(\ddot{\gamma}^\nu(ct) + \dot{\gamma}^\mu(t)\dot{\gamma}^\rho(t)\Gamma^\nu_{\mu\rho}(\gamma(ct)) \\ &= c^2 D_t\dot{\gamma}^\nu(ct) = 0\end{aligned}$$

and conclude that $\tilde{\gamma} = \gamma_{cX}$ by the uniqueness property of geodesics.

The statement (ii) immediately follows since: $\mathrm{Exp}_p(tX) = \gamma_{tX}(1) = \gamma_X(t)$.

We turn to (iii). Let $X \in \mathcal{E}_p$. Then the domain of γ_X includes $[0,1]$ by definition. By (ii), we have that for $0 \le t \le 1$, $\mathrm{Exp}_p(tX) = \gamma_{tX}(1) = \gamma_X(t)$ is well-defined, so $tX \in \mathcal{E}_p$. From Picard–Lindelöf it follows moreover that there exists an $r > 0$ such that for all $X \in T_p\mathcal{M}$ with $|X| = 1$, γ_X is well defined in $[0, r]$. By (ii), this means that Exp is well-defined on $B_r(0) \subset \mathcal{E}_p$.

Finally, smoothness of Exp_p follows from smoothness of the metric g and the continuous dependence of the solution to the ODE on initial data, applied also to higher-order time derivatives of γ. □

We will use the map Exp_p to construct a particularly convenient coordinate chart.

Proposition A.6. *For any $p \in \mathcal{M}$, there exists a neighbourhood V of $0 \in T_p\mathcal{M}$ and a neighbourhood U of p in $\mathcal{M}$ such that*

$$\mathrm{Exp}_p : V \to U$$

is a diffeomorphism.

The set U is called a *normal neighbourhood of p*.

Proof. This follows from the inverse function theorem, once we establish invertibility of $(\mathrm{Exp}_p)_* : T_p\mathcal{M} \cong T_0(T_p\mathcal{M}) \to T_p\mathcal{M}$. Let $X \in T_p\mathcal{M}$ and let $\delta : \mathbb{R} \to T_p\mathcal{M}$ be defined as $\delta(t) = tX$. Then $X = \dot{\delta}(0) \in T_0(T_p\mathcal{M})$. Hence,

$$(\mathrm{Exp}_p)_*(X) = \frac{d}{dt}|_{t=0}(\mathrm{Exp} \circ \delta)(t) = \frac{d}{dt}|_{t=0}\mathrm{Exp}(tX) = \frac{d}{dt}|_{t=0}\gamma_X(t) = X.$$

So $(\mathrm{Exp}_p)_*$ is the identity map and is thus clearly invertible. □

Let $p \in T_p\mathcal{M}$ and let $\{e_\mu\}$ be an orthonormal basis on T_pM. Then $E : \mathbb{R}^n \to T_p\mathcal{M}$, $E(x^1, \ldots, x^n) = x^\mu e_\mu$ defines an isomorphism.

We refer to $\mathrm{Exp}(B_r(0))$ as the *geodesic ball* of radius r centred at p.

Definition A.3. *Let U be a normal neighbourhood of $p \in \mathcal{M}$. The map $\psi : U \to \mathbb{R}^n$, $\psi = E^{-1} \circ \mathrm{Exp}_p^{-1} : U \to \mathbb{R}^n$ defines a coordinate chart. The corresponding coordinates $x^\mu = \psi^\mu$ are called* normal coordinates.

Proposition A.7. *Normal coordinates satisfy the following properties:*

(i) *Let $X = X^\mu e_\mu \in T_p\mathcal{M}$. Then γ_X in normal coordinates is represented by:*

$$\gamma_V(t) = t(X^1, \ldots, X^n).$$

for all $t \in \mathbb{R}$ such that $\mathrm{Exp}_p(tX) \in U$.

(ii) *The coordinates of p are $(0, \ldots, 0)$.*

(iii) *The components of g at p are equal to the components in Cartesian coordinates of the Euclidean metric in the Riemannian case or the Minkowski metric in the Lorentzian case, i.e. $g_{\mu\nu} = \delta_{\mu\nu}$ (Riemannian) and $g_{\mu\nu} = m_{\mu\nu}$ (Lorentzian).*

(iv) *The derivatives of $g_{\mu\nu}$ vanish at p: $\partial_\rho g_{\mu\nu}(p) = 0$ with respect to normal coordinates. In particular, $\Gamma^\rho_{\mu\nu}(p) = 0$.*

Proof. Property (i) follows from the fact that $\psi(\gamma_X(t)) = \psi(\mathrm{Exp}_p(tX)) = E^{-1}(tX) = t(X^1, \dots, X^n)$. Similarly, (ii) follows from $\psi(p) = \psi(\mathrm{Exp}_p(0)) = (0, \dots, 0)$.

Consider now (iii). We have that $g_{\mu\nu}(p) = g_p(\partial_\mu|_p, \partial_\nu|_p)$, where $\partial_\mu|_p \in T_p\mathcal{M}$ is the basis vector field associated to the normal coordinates $\{x^\mu\}$. By construction, $\partial_\mu|_p = \dot\gamma_{e_\mu}(0) = e_\mu$. Hence, (iii) follows from the assumption that $\{e_\mu\}$ form an orthonormal basis of $T_p\mathcal{M}$ with respect to $g(p)$.

Finally, we will show (iv). We first show that the Christoffel symbols must vanish. This follows from the geodesic equation expressed in normal coordinates: let $X \in T_p\mathcal{M}$, then

$$0 = (D_t\dot\gamma_X)^\nu(0) = \ddot\gamma^\mu(0) + \Gamma^\nu_{\mu\rho}(p)X^\mu X^\rho = \Gamma^\nu_{\mu\rho}(p)X^\mu X^\rho,$$

by (i). Since X was arbitrary, it follows immediately that $\Gamma^\nu_{\mu\mu}(p) = 0$ for all μ. By the symmetry of $\Gamma^\nu_{\mu\rho}(p)$ in its lower two indices, one can also show that $\Gamma^\nu_{\mu\rho}(p) = 0$ for all μ, ρ (Exercise). To conclude that partial derivatives of $g_{\mu\nu}$ vanish, we use the following identity at p:

$$\begin{aligned} 0 &= g_{\mu\sigma}\Gamma^\sigma_{\nu\rho} + g_{\nu\sigma}\Gamma^\sigma_{\mu\rho} = \frac{1}{2}g_{\mu\sigma}(g^{-1})^{\sigma\alpha}(\partial_\nu g_{\rho\alpha} + \partial_\rho g_{\nu\alpha} - \partial_\alpha g_{\nu\rho}) + \mu \leftrightarrow \nu \\ &= \frac{1}{2}(\partial_\nu g_{\rho\mu} + \partial_\rho g_{\nu\mu} - \partial_\mu g_{\nu\rho}) + \mu \leftrightarrow \nu \\ &= \partial_\rho g_{\nu\mu}. \end{aligned}$$

□

Remark A.2. *One may compare the existence of normal coordinate in a neighbourhood of every point to Darboux's Theorem in symplectic geometry, which states that on a symplectic manifold $(\mathcal{M}, \omega)$ of dimension $2n$ and $p \in \mathcal{M}$, here exist coordinates $(x^1, \dots, x^n, y^1, \dots, y^n)$ in neighbourhood of p, such that $\omega = \sum_{i=1}^n dx^i \wedge dy^i$. The key difference for $(\mathcal{M}, g)$, however, is that the identities $g_{\mu\nu} = m_{\mu\nu}$ and $\partial_\rho g_{\mu\nu} = 0$ only necessarily hold <u>at</u> p and not in a full neighbourhood of p. Related to this, we will see that second-order derivatives of $g_{\mu\nu}$ can not all be made to vanish in general.*

Remark A.3. *Let $\gamma : (-\epsilon, \epsilon) \to \mathcal{M}$ be a geodesic with $\gamma(0) = p$. With a little bit more work and for $\epsilon > 0$ suitably small, it is possible to construct a coordinate chart in a neighbourhood U of $\gamma(-\epsilon, \epsilon)$, such that $g_{\mu\nu}(q) = \Gamma^\nu_{\mu\nu}(q) = \partial_\rho g_{\mu\nu}(q) = 0$ for all $q \in \gamma(-\epsilon, \epsilon)$. The corresponding coordinates are called* Fermi normal coordinates.

If we interpret timelike geodesics in Lorenzian manifolds as representing free falling observers in spacetime, carrying orthogonal measuring rods, the existence of Fermi normal coordinates may be thought of as providing a precise mathematical formulation of the equivalence principle *in general relativity. This, loosely formulated, states that non-gravitational experiments performed by free-falling observers at sufficiently small time and length scales cannot be distinguished from those performed by non-accelerating observers in Minkowski spacetime.*

A.2 Curvature

Let $(\mathcal{M}, g)$ be a Riemannian or Lorentzian manifold with Levi–Civita connection.

We introduce a map that describes an *intrinsic*[28] notion of curvature of $(\mathcal{M}, g)$.

Definition A.4. *The* Riemann curvature endomorphism *is defined as the map:*

$$\begin{aligned} \mathrm{Riem} &: \Gamma(T\mathcal{M}) \times \Gamma(T\mathcal{M}) \times \Gamma(T\mathcal{M}) \to \Gamma(T\mathcal{M}) \\ \mathrm{Riem}(X, Y)Z &:= \nabla_X\nabla_Y Z - \nabla_Y\nabla_X Z - \nabla_{[X,Y]}Z. \end{aligned}$$

[28] Independent of how the manifold may be embedded in some larger manifold.

The proposition below shows that we can interpret Riem as a $(1,3)$-tensor field, which we will call the *Riemann curvature tensor*.

Proposition A.8. $\text{Riem} \in \mathcal{T}^{(1,3)}(\mathcal{M}) = \Gamma(T^*\mathcal{M} \otimes T^*\mathcal{M} \otimes T^*\mathcal{M} \otimes T\mathcal{M})$

Proof. We can characterize $(1,3)$ tensor fields as maps on $\Gamma(T\mathcal{M}) \times \Gamma(T\mathcal{M}) \times \Gamma(T\mathcal{M}) \to \Gamma(T\mathcal{M})$ that are multilinear over $C^\infty(\mathcal{M})$. It is immediate that the map is multilinear over $\mathbb{R}$, by the linearity of the operations in its definition. Exercise: Show that

$$\begin{aligned}\text{Riem}(fX, Y)Z =& f\text{Riem}(X, Y)Z,\\ \text{Riem}(X, fY)Z =& f\text{Riem}(X, Y)Z,\\ \text{Riem}(X, Y)(fZ) =& f\text{Riem}(X, Y)Z,\end{aligned}$$

for all $f \in C^\infty(\mathcal{M})$ and $X, Y, Z \in \Gamma(T\mathcal{M})$. □

We denote the components of Riem with respect to a basis on $T_p\mathcal{M}$ by $R^\sigma{}_{\mu\nu\rho}$, with $\text{Riem}(X,Y)Z = R^\sigma{}_{\mu\nu\rho}Z^\mu X^\nu Y^\rho \partial_\sigma$. In particular, with respect to a coordinate basis we have that:

$$\begin{aligned}\text{Riem}(\partial_\nu, \partial_\rho)\partial_\mu &= \nabla_{\partial_\nu}\nabla_{\partial_\rho}\partial_\mu - \nabla_{\partial_\rho}\nabla_{\partial_\nu}\partial_\mu\\ &= \nabla_{\partial_\nu}(\Gamma^\sigma_{\rho\mu}\partial_\sigma) - \nabla_{\partial_\rho}(\Gamma^\sigma_{\nu\mu}\partial_\sigma)\\ &= \partial_\nu\Gamma^\sigma_{\rho\mu}\partial_\sigma - \partial_\rho\Gamma^\sigma_{\nu\mu}\partial_\sigma + \Gamma^\sigma_{\rho\mu}\Gamma^\alpha_{\nu\sigma}\partial_\alpha - \Gamma^\sigma_{\nu\mu}\Gamma^\alpha_{\rho\sigma}\partial_\alpha\end{aligned}$$

Hence,

$$R^\sigma{}_{\mu\nu\rho} = \partial_\nu\Gamma^\sigma_{\rho\mu} - \partial_\rho\Gamma^\sigma_{\nu\mu} + \Gamma^\kappa_{\rho\mu}\Gamma^\sigma_{\nu\kappa} - \Gamma^\kappa_{\nu\mu}\Gamma^\sigma_{\rho\kappa}.$$

In particular, with respect to normal coordinates at $p \in \mathcal{M}$, we have that

$$R^\sigma{}_{\mu\nu\rho}(p) = \partial_\nu\Gamma^\sigma_{\rho\mu}(p) - \partial_\rho\Gamma^\sigma_{\nu\mu}(p).$$

We will also refer to the $(0,4)$-tensor field $\text{Riem}^\flat$ with components $R_{\mu\nu\rho\sigma}$ as the Riemann curvature tensor.

Definition A.5. *The* Ricci tensor *is defined as the* $(0,2)$*-tensor field* Ric *with components* $R_{\mu\nu}$*, defined as follows:*

$$R_{\mu\nu} = R^\sigma{}_{\mu\sigma\nu}.$$

Definition A.6. *The* Ricci scalar $R \in C^\infty(\mathcal{M})$ *is defined as follows:*

$$R = (g^{-1})^{\mu\nu}R_{\mu\nu}.$$

The Riemann tensor and its contractions are natural quantities to consider on $(\mathcal{M}, g)$ because they are invariant under isometries, which are diffeomorphisms $\Phi : \mathcal{M} \to \widetilde{\mathcal{M}}$, where $(\mathcal{M}, g)$ and $(\widetilde{\mathcal{M}}, \widetilde{g})$ are Riemannian/Lorentzian manifolds, such that $\Phi^*\widetilde{g} = g$.

Proposition A.9. *Let* $(\mathcal{M}, g)$ *and* $(\widetilde{\mathcal{M}}, \widetilde{g})$ *be Riemannian/Lorentzian manifolds with Riemann curvature tensors* Riem *and* $\widetilde{\text{Riem}}$*, respectively. Let* $\Phi : \mathcal{M} \to \widetilde{\mathcal{M}}$ *be an isometry. Then*

$$\begin{aligned}\widetilde{\text{Riem}}(\Phi_*X, \Phi_*Y)\Phi_*Z &= \Phi_*(\text{Riem}(X, Y, Z)),\\ \Phi^*\widetilde{\text{Riem}} &= \text{Riem}.\end{aligned}$$

Proof. See exercises on Problem Sheet 12. □

The Riemann curvature tensor enjoys various symmetry properties.

Proposition A.10. *With respect to an arbitrary coordinate chart, the components of the Riemann tensor satisfy:*

(i) $R^\sigma{}_{\mu(\nu\rho)} = 0$,

(ii) $R^{\sigma}{}_{[\mu\nu\rho]} = 0$,

(iii) $\nabla_{[\alpha} R_{\sigma\mu]\nu\rho} = 0$ *(Bianchi identity)*,

(iv) $R_{\sigma\mu\nu\rho} = R_{\nu\rho\sigma\mu}$,

(v) $R_{(\sigma\mu)\nu\rho} = 0$.

Proof. Omitted □

From the above symmetry properties, we can deduce symmetry properties at the level of the Ricci tensor and Ricci scalar. We first introduce the Einstein tensor.

Definition A.7. *The Einstein tensor G is a $(0,2)$-tensor field on $\mathcal{M}$ defined as follows:*

$$G = \mathrm{Ric} - \frac{1}{2} R g.$$

Corollary A.11. *The Ricci and Einstein tensors are symmetric and, with respect to an arbitrary coordinate chart, G satisfies the* contracted Bianchi identity

$$\nabla^{\mu} G_{\mu\nu} = 0.$$

Proof. Symmetry of G follows immediately from symmetry of Ric. Recall,

$$R_{\mu\nu} = R^{\sigma}{}_{\mu\sigma\nu} = (g^{-1})^{\sigma\alpha} R_{\alpha\mu\sigma\nu}.$$

By property (iv) of Proposition A.10, we have that

$$(g^{-1})^{\sigma\alpha} R_{\alpha\mu\sigma\nu} = (g^{-1})^{\sigma\alpha} R_{\sigma\nu\alpha\mu} = R_{\nu\mu}.$$

To derive the contracted Bianchi identity, we combine (i) and (iii) to infer that $R^{\sigma}{}_{\mu\nu\rho} = R^{\sigma}{}_{[\mu\nu]\rho}$ and

$$\nabla_{\alpha} R_{\sigma\mu\nu\rho} + \nabla_{\sigma} R_{\mu\alpha\nu\rho} + \nabla_{\mu} R_{\alpha\sigma\nu\rho} = 0.$$

Now we contract the above identity with $(g^{-1})^{\sigma\nu}(g^{-1})^{\mu\rho}$ to obtain:

$$\begin{aligned} 0 &= (g^{-1})^{\sigma\nu}(g^{-1})^{\mu\rho} \nabla_{\alpha} (R_{\sigma\mu\nu\rho} + \nabla_{\sigma} R_{\mu\alpha\nu\rho} + \nabla_{\mu} R_{\alpha\sigma\nu\rho}) \\ &= \nabla_{\alpha} R - \nabla^{\nu} R_{\alpha\nu} - \nabla^{\rho} R_{\alpha\rho} \\ &= \nabla_{\alpha} R - 2\nabla^{\nu} R_{\alpha\nu} \\ &= -2\nabla^{\nu} G_{\alpha\nu}. \end{aligned}$$

□