NOTES ON CLASSICAL MECHANICS

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Last updated: January 16, 2023

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PREFACE

Although classical, the subject of mechanical systems continues to be important in modern research on differential equations, with applications to the studies of ODEs, Lagrangian PDEs, and Hamiltonian PDEs. In each application, the general theorems of mechanics serve as overarching principles while the details for the particular example at hand are worked out. Nevertheless, the subject of classical mechanics is often elided in today's physics curricula in order to make way for more active fields of research. I found this particularly inconvenient as a student learning mathematical tools originating from classical mechanics, as neither the physics nor math departments taught the corresponding physical motivation and intuition. Consequently, these notes are the product of a personal effort to collect these mathematical ideas and connect them to their physical inspiration.

The first objective of these notes is to present the core theory of classical mechanics palatable to mathematicians. The presentation is intended to be self-contained and mathematically rigorous, while maintaining the example-driven physical mindset in order to cultivate intuition. From a physics viewpoint however, this excludes many topics that commonly appear in a first-year graduate course on the subject (e.g. rigid bodies). For a thorough study of the physical theory, techniques, and examples of classical mechanics, we refer the reader to the classic physics texts [Arn89, Gol51, LL76].

The second objective of these notes is to develop the resultant mathematical theory alongside the physical inspiration, and to recognize the physical system as an example. These mathematical tools are foundational in the theory of ODEs, and they are still commonly found throughout modern mathematics. Note that this does not include the rich field of mathematical *methods* used in physics, for which we refer the reader to the excellent mathematics texts [AKN06, SM95, MZ05].

In order to focus on mathematical tools which arose from mechanics, we will assume the reader possesses a beginner graduate or advanced undergraduate understanding of mathematics. Specifically, we assume the reader is familiar with multivariate real analysis throughout, with manifolds and tangent bundles in Part II, and with differential forms in Part III. Moreover, we will almost always work in the class of smooth (i.e. infinitely differentiable) functions. Although many of the results hold under weaker assumptions, we choose to focus on the proofs in the smooth case in order to highlight the physical motivation.

PART I

NEWTONIAN MECHANICS

The Newtonian framework is the most fundamental interpretation of the motion of mechanical systems. The physical theory is based on a few empirical observations which are taken as axioms, among which are Newton's equations of motion. The resulting differential equations inherit special properties from their corresponding physical systems. Extracting mathematical statements about the behavior of solutions from these properties illustrates some classical tools from the theory of ODEs. Along the way, we will also identify the key mathematical ideas that will allow us to include more general systems in the proceeding parts.

CHAPTER 1

NEWTON'S EQUATIONS

We begin the physical theory with the essential empirical observations and its immediate consequences. The material for this chapter is based on [Arn89, Ch. 1], [AKN06, Ch. 1], and [Gol51, Ch. 1].

1.1. Empirical assumptions

Classical mechanics is the study of the motion of particles in Euclidean space $\mathbb{R}^d$. A **particle** (or **point mass**) consists of two pieces of information: the body's **mass** $m > 0$ and its **position** $\mathbf{x} \in \mathbb{R}^d$. This model for physical objects neglects the object's spatial dimensions. Given a system of N particles with positions $\mathbf{x}_i \in \mathbb{R}^d$, the collection of all possible positions $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_N)$ constitutes the **configuration space** $\mathbb{R}^d \times \cdots \times \mathbb{R}^d = \mathbb{R}^{Nd}$, whose dimension Nd is the system's **degrees of freedom**.

The evolution of a system is described by the particles' **trajectories**, N maps $\mathbf{x}_i : I \to \mathbb{R}^d$ for $I \subset \mathbb{R}$ an interval, which together constitute the motion of the system. In order to determine the system's evolution we will use the **velocity** $\dot{\mathbf{x}}_i$, **acceleration** $\ddot{\mathbf{x}}_i$, and **momentum**

$$\mathbf{p}_i = m_i \dot{\mathbf{x}}_i \tag{1.1}$$

of the ith particle. (We use the notation $\dot{f} = \frac{\mathrm{d}f}{\mathrm{d}t}$ for time derivatives.) The positions and momenta together span the **phase space** $\mathbb{R}^{Nd} \times \mathbb{R}^{Nd}$, whose dimension $2Nd$ is always twice the degrees of freedom. We will refer to the trajectories of the system plotted in phase space as the system's **phase portrait**.

Newton's principle of determinacy is the experimental observation that the initial state of a Newtonian system—all the positions $\mathbf{x}(t_0)$ and velocities $\dot{\mathbf{x}}(t_0)$ at some moment $t_0 \in \mathbb{R}$ in time—uniquely determines the system's motion. We formulate this mathematically as follows:

Definition 1.1 (Newton's principle of determinacy)**.** A **Newtonian system** is given by N particles and a function $\mathbf{F} : \mathbb{R} \times (\mathbb{R}^{Nd} \setminus \Delta) \times \mathbb{R}^{Nd} \to \mathbb{R}^{Nd}$, called the **force**, such that

$$\dot{\mathbf{p}} = \mathbf{F}(t, \mathbf{x}, \dot{\mathbf{x}}). \tag{1.2}$$

Here, $\Delta = \bigcup_{i<j} \{\mathbf{x}_i = \mathbf{x}_j\}$ is the union of diagonals, so that we do not consider two particles occupying the same position.

The system of equations (1.2) are called **Newton's equations** (or **Newton's second law**). Unless otherwise noted, we will always assume the particle masses m_i are constant. In this case, (1.2) takes the form

$$m_i \ddot{\mathbf{x}}_i = \mathbf{F}_i(t, \mathbf{x}, \dot{\mathbf{x}}) \quad \text{for } i = 1, \dots, N. \tag{1.3}$$

Newton's equations are commonly stated in terms of the momentum $\mathbf{p}$ instead of the velocity $\dot{\mathbf{x}}$ because experimentally we can observe that a particle's acceleration by a force is inversely proportional to its mass.

In mathematics, it is common practice to reduce a system of N second-order ordinary differential equations (ODEs) on configuration space to first-order. To do this, we group the equations (1.1) for $\dot{\mathbf{x}}$ together with the equations (1.2) for $\dot{\mathbf{p}}$ to obtain a system of $2N$ first-order ODEs on phase space. For initial conditions, we then take the positions $\mathbf{x}(t_0)$ and momenta $\mathbf{p}(t_0)$ at some time $t_0 \in \mathbb{R}$. For convenience, we may assume that $t_0 = 0$ after replacing the variable t by $t - t_0$.

Unless otherwise stated, we will always assume that the force $\mathbf{F}$ is smooth (i.e. infinitely differentiable) on $\mathbb{R} \times (\mathbb{R}^{Nd} \smallsetminus \Delta) \times \mathbb{R}^{Nd}$. It then follows (cf. Theorem A.5) that there exists a unique solution $\mathbf{x}(t)$ to the system of differential equations (1.3) for any initial state. However, the solution is only guaranteed to exist on a short time interval, and in general may not be able to be extended for all time (cf. Example A.4). From experience though, we expect that for naturally occurring mechanical systems that the time interval of existence can be extended to all of $\mathbb{R}$. Indeed, most of our mathematical statements will include a premise that ensures that the solutions to our mathematical model (1.3) exist for all time.

We will often impose one additional assumption: that the physical laws governing the system's motion is independent of the choice of coordinates and origin on $\mathbb{R}^d$. A transformation $\mathbb{R}_t \times \mathbb{R}^d \to \mathbb{R}_t \times \mathbb{R}^d$ is **Galilean** provided that it is an affine transformation (a linear transformation and a translation) that preserves time intervals and for any fixed $t \in \mathbb{R}$ is an isometry of $\mathbb{R}^d$. In other words, if we write $g(t, \mathbf{x}) = (t', \mathbf{x}')$ then for each $t \in \mathbb{R}$ the function $\mathbf{x}'$ is an orthogonal transformation and a translation. It is straightforward to check that the set of Galilean transformations forms a group under function composition.

Example 1.2. The following are all Galilean transformations:

(a) Translations: $g_1(t, \mathbf{x}) = (t + t_0, \mathbf{x} + \mathbf{x}_0)$ for some fixed $\mathbf{x}_0 \in \mathbb{R}^d$, $t_0 \in \mathbb{R}$.

(b) Rotations and reflections: $g_2(t, \mathbf{x}) = (t, A\mathbf{x})$ for some fixed orthogonal transformation $A \in O(d)$.

(c) Galilean boosts: $g_3(t, \mathbf{x}) = (t, \mathbf{x} + \mathbf{v}t)$ for some fixed velocity $\mathbf{v} \in \mathbb{R}^d$.

In fact, these examples generate the entire Galilean group (cf. Exercise 1.1). **Galileo's principle of relativity** is the experimental observation that for an isolated system there exists a **reference frame**—a choice of origin and coordinate axes for $\mathbb{R}^d$—that is invariant under any Galilean transformation.

Such a reference frame is called **inertial**, and the principle also asserts that all coordinate systems in uniform motion with constant velocity with respect to an inertial frame must also be inertial. (This is observed, for example, in a car traveling at constant velocity and noting that motion inside the car is as if the car were at rest.) We formulate this mathematically as follows:

Definition 1.3 (Galileo's principle of relativity)**.** A Newtonian system is **isolated** if there exists a reference frame so that Newton's equations (1.2) are invariant under any Galilean transformation.

Physically, this is requiring that the ambient space is both homogeneous and isotropic and that time is homogeneous. Geometrically, this principle requires that if we apply a Galilean transformation to a phase portrait, then the resulting graph still consists of trajectories.

If Newton's equations (1.2) hold in an inertial coordinate system, then they must be invariant with respect to the Galilean group. Let $\mathbf{x}(t)$ denote a solution in these coordinates. Applying the Galilean group generators of Example 1.2, we find the following conditions on $\mathbf{F}_i$:

(a) Translation invariance: $\mathbf{F}_i(t, \mathbf{x}, \dot{\mathbf{x}}) \equiv \mathbf{F}_i(\mathbf{x}_j - \mathbf{x}_k, \dot{\mathbf{x}})$.

(b) Rotation and reflection invariance: $\mathbf{F}_i(A\mathbf{x}, A\dot{\mathbf{x}}) = A\mathbf{F}_i(\mathbf{x}, \dot{\mathbf{x}})$ for $A \in O(d)$.

(c) Boost invariance: $\mathbf{F}_i(\mathbf{x}_j - \mathbf{x}_k, \dot{\mathbf{x}}) \equiv \mathbf{F}_i(\mathbf{x}_j - \mathbf{x}_k, \dot{\mathbf{x}}_j - \dot{\mathbf{x}}_k)$.

Note that the third type of transformation in Example 1.2 changes neither $\ddot{\mathbf{x}}$ nor $\mathbf{x}_i - \mathbf{x}_j$.

Proposition 1.4 (Newton's first law, special case)**.** *For an isolated Newtonian system of one particle, the particle's acceleration in an inertial coordinate system vanishes. In particular, the motion is* ***rectilinear****: uniform in time with constant velocity.*

Proof. Taking $N = 1$, the conditions (a)–(c) above require that $\mathbf{F}$ is independent of $\mathbf{x}$, $\dot{\mathbf{x}}$, t and is rotationally invariant. Therefore $\mathbf{F} \equiv 0$. □

1.2. Kinetic energy

The **kinetic energy** of the ith particle and the **total kinetic energy** are given by

$$K_i = \tfrac{1}{2} m_i |\dot{\mathbf{x}}_i|^2 = \tfrac{1}{2m_i} |\mathbf{p}_i|^2, \qquad K = \sum_{i=1}^{N} K_i \tag{1.4}$$

respectively. From experience, we know that the magnitude of the velocity and hence the kinetic energy can be increased and decreased by the force $\mathbf{F}_i$ acting on the ith particle, depending on the force's magnitude and direction. This is measured through the **work** W_i done by the force $\mathbf{F}_i$ on the ith particle from time 0 to t, defined by

$$W_i = \int_{\mathbf{x}(0)}^{\mathbf{x}(t)} \mathbf{F}_i \cdot \, \mathrm{d}\mathbf{s}_i = \int_0^t \mathbf{F}_i(\mathbf{x}(\tau)) \cdot \dot{\mathbf{x}}(\tau) \, \mathrm{d}\tau.$$

(We use $\mathrm{d}\mathbf{s}_i$ to denote the line element of the trajectory $\mathbf{x}_i(t)$, and so the second equality is the definition of path integration.) Although work is measured in the physical space $\mathbb{R}^d$, the **total work**

$$W = \int_{\mathbf{x}(0)}^{\mathbf{x}(t)} \mathbf{F} \cdot \mathrm{d}\mathbf{s}$$

is measured on configuration space $\mathbb{R}^{Nd}$.

The net change in kinetic energy is due to the work done by the force $\mathbf{F}$ on the path $\mathbf{x}(t)$ in configuration space:

Proposition 1.5. *The increase in total kinetic energy is equal to the total work.*

Proof. Differentiating the kinetic energy (1.4), we obtain

$$\dot{K} = \sum_{i=1}^{N} m_i \dot{\mathbf{x}}_i \cdot \ddot{\mathbf{x}}_i = \sum_{i=1}^{N} \dot{\mathbf{x}}_i \cdot \mathbf{F}_i = \dot{\mathbf{x}} \cdot \mathbf{F} \tag{1.5}$$

by Newton's equations (1.3). Integrating, we have

$$K(t) - K(0) = \int_0^t \dot{K}\, \mathrm{d}t = \int_0^t \dot{\mathbf{x}} \cdot \mathbf{F}\, \mathrm{d}\tau = \int_{\mathbf{x}(0)}^{\mathbf{x}(t)} \mathbf{F} \cdot \mathrm{d}\mathbf{s} = W. \qquad \square$$

1.3. Potential energy

For some systems there is also a potential energy. In physics, a Newtonian system is called **conservative** if the force $\mathbf{F}(t, \mathbf{x}, \dot{\mathbf{x}}) \equiv \mathbf{F}(\mathbf{x})$ depends only on the positions $\mathbf{x}$ and if the total work along any path connecting two points $\mathbf{y}, \mathbf{z}$ in configuration space,

$$W = \int_{\mathbf{y}}^{\mathbf{z}} \mathbf{F}(\mathbf{s}) \cdot \mathrm{d}\mathbf{s},$$

is independent of the path chosen for the line integral. (Note that the line integral path is allowed to be arbitrary, and is not limited to trajectories.) This independence is equivalent to the work around any simple closed path vanishing, since two paths with the same endpoints can be concatenated to form one closed path.

One way for this to be satisfied is if there is a **potential energy**, a function V such that $\mathbf{F} = -\nabla V$. Indeed, if this is the case, then by the fundamental theorem of calculus we have

$$W = -\int_{\mathbf{y}}^{\mathbf{z}} \nabla V(\mathbf{s}) \cdot \mathrm{d}\mathbf{s} = -V(\mathbf{z}) + V(\mathbf{y})$$

for all paths connecting $\mathbf{y}$ to $\mathbf{z}$.

Example 1.6. If the interaction forces depend only on particle distances:

$$\mathbf{F}_i = \sum_{j=1}^{N} \mathbf{F}_{ij}, \qquad \mathbf{F}_{ij} = f_{ij}\big(|\mathbf{x}_i - \mathbf{x}_j|\big)\mathbf{e}_{ij}, \qquad \mathbf{e}_{ij} = \frac{\mathbf{x}_j - \mathbf{x}_i}{|\mathbf{x}_j - \mathbf{x}_i|},$$

then the system is conservative with potential energy

$$V = \sum_{i<j} V_{ij}, \qquad V_{ij} = \int f_{ij}(r)\,\mathrm{d}r.$$

In fact, every conservative system must have a potential energy:

Proposition 1.7. *A Newtonian system is conservative if and only if there exists a potential energy, i.e. a smooth function* $V : \mathbb{R}^{Nd} \setminus \Delta \to \mathbb{R}$ *such that* $\mathbf{F} = -\nabla V$.

Proof. First suppose that the total work integral is path independent. Fix some $\mathbf{x}_0 \in \mathbb{R}^{Nd} \setminus \Delta$. Then the line integral

$$V(\mathbf{x}) = -\int_{\mathbf{x}_0}^{\mathbf{x}} \mathbf{F}(\mathbf{s}) \cdot \mathrm{d}\mathbf{s}$$

is well-defined as a function of $\mathbf{x}$, because its value is independent of the choice of path from $\mathbf{x}_0$ to $\mathbf{x}$. We then have $\mathbf{F} = -\nabla V$ by the fundamental theorem of calculus.

Conversely, if there is a potential energy V, then the fundamental theorem of calculus tells us that

$$\int_{\mathbf{x}_0}^{\mathbf{x}} \mathbf{F} \cdot \mathrm{d}\mathbf{s} = -\int_{\mathbf{x}_0}^{\mathbf{x}} \nabla V(\mathbf{s}) \cdot \mathrm{d}\mathbf{s} = -V(\mathbf{x}) + V(\mathbf{x}_0).$$

That is, the work is independent of the path. □

In Proposition 1.7, it is assumed that $\mathbf{F}$ and V are defined on all of $\mathbb{R}^{Nd} \setminus \Delta$. The statement does not hold for arbitrary open subsets of the configuration space $\mathbb{R}^{Nd}$:

Example 1.8. Consider the vector field

$$\mathbf{F}(x, y) = \left(\frac{y}{x^2 + y^2}, -\frac{x}{x^2 + y^2}\right)$$

on $\mathbb{R}^2 \setminus \{(0, 0)\}$. This is the negative gradient of the angle coordinate, which is defined on all of $\mathbb{R}^2 \setminus \{(0, 0)\}$ unlike the angle coordinate alone. Consequently, by the fundamental theorem of calculus the work done on a particle traveling around any simple closed curve not containing the origin is zero. Conversely, the work done on a particle traveling once clockwise about the unit circle is 2π, which reflects the fact that we cannot define a single-valued angle coordinate on all of $\mathbb{R}^2 \setminus \{(0, 0)\}$. Consequently, the system consisting of one particle subject to this force is an example of a nonconservative force.

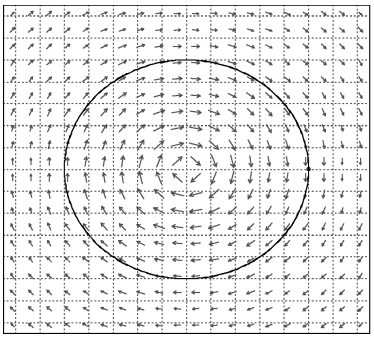


Figure 1.1: Configuration space for the system of Example 1.8.

Example 1.8 shows that unlike $\mathbb{R}^2$, a curl-free vector field on $\mathbb{R}^2 \setminus \{(0,0)\}$ is not necessarily gradient field. Consequently, the fact that Proposition 1.7 holds on $\mathbb{R}^{Nd} \setminus \Delta$ may initially be surprising. To understand why this works, take $d = 3$, fix $N - 1$ particles, and consider only moving the ith particle. Let S be a smooth 2-dimensional surface in $\mathbb{R}^3$ with boundary. Using Green's theorem we write

$$0 = \int_{\partial S} \mathbf{F}_i \cdot \, \mathrm{d}\mathbf{s}_i = \int_S (\nabla_i \times \mathbf{F}_i) \cdot \mathbf{n} \, \mathrm{d}A,$$

where $\mathbf{n}$ is a unit vector field that is perpendicular to S. For this to hold for all such surfaces S, then we must have $\nabla_i \times \mathbf{F}_i \equiv 0$. So the definition of a conservative force is an integral formulation of $\mathbf{F}_i$ being curl-free on *all of* $\mathbb{R}^3$, which avoids the issue of $\mathbf{F}_i$ not being defined on $\bigcup_{j \neq i} \{\mathbf{x}_j\}$. As the domain is all of $\mathbb{R}^3$, we know that $\nabla \times \mathbf{F}_i \equiv 0$ implies $\mathbf{F}_i = -\nabla V_i(\mathbf{x}_i)$, but with the caveat that our potential V_i may not be defined on $\bigcup_{j \neq i} \{\mathbf{x}_j\}$ because $\mathbf{F}$ is not defined on the diagonals Δ.

A similar argument also applies to dimensions $d \neq 3$ using differential forms: if $\mathbf{F}_i$ is conservative then $\mathbf{F}_i$ is a closed 1-form (i.e. $\mathrm{d}\mathbf{F}_i \equiv 0$) on all of $\mathbb{R}^d$. This then implies that $\mathbf{F}_i$ is exact (i.e. $\mathbf{F}_i = -\mathrm{d}V_i$), although the 0-form V_i may not be defined on $\bigcup_{j \neq i} \{\mathbf{x}_j\}$. In comparison, the 1-form $\mathbf{F}_i$ of Example 1.8 is closed on $\mathbb{R}^2 \setminus \{0\}$ (if $S \subset \mathbb{R}^2 \setminus \{0\}$ then the work around ∂S vanishes), but it is not closed on all of $\mathbb{R}^2$.

1.4. Total energy

We now have two notions of mechanical energy: kinetic and potential. Their sum $E = K + V$ is the system's **total energy**, and it is conserved under the dynamics:

Proposition 1.9 (Conservation of energy)**.** *For a conservative system, the total energy E is conserved: $E(t) = E(0)$ for all $t \in \mathbb{R}$.*

Proof. By the computation (1.5) and Newton's equations (1.3), we have

$$\dot{E} = \dot{K} + \nabla V \cdot \dot{\mathbf{x}} = \dot{\mathbf{x}} \cdot \mathbf{F} - \mathbf{F} \cdot \dot{\mathbf{x}} = 0.$$

Therefore $E(t)$ must be constant. □

The conservation of energy is associated with the system's time symmetry. Clearly a conservative system is automatically time-independent by definition. As we will see later, converses of this statement is also true (cf. section 2.4, Proposition 4.11, Exercise 4.8, and Proposition 7.3).

In section 2.2 we will explore the implications of energy conservation in greater detail, but as immediate consequences we record a couple of statements regarding the global existence of solutions. The best case scenario is when the potential is coercive at infinity:

Corollary 1.10. *If a conservative system has a smooth nonnegative potential energy $V(\mathbf{x})$ that satisfies $V(\mathbf{x}) \to +\infty$ as $|\mathbf{x}| \to \infty$, then solutions exist for all time.*

Proof. Fix initial data and let E_0 denote the corresponding initial energy. By conservation of energy (Proposition 1.9), we know that the solution is confined to the region $\{(\mathbf{x}, \dot{\mathbf{x}}) : \frac{1}{2}|\dot{\mathbf{x}}|^2 + V(\mathbf{x}) = E_0\}$ for as long as it exists. This region is contained in the set $\{\frac{1}{2}|\dot{\mathbf{x}}|^2 \leq E_0\} \cap \{V(\mathbf{x}) \leq E_0\}$, which is bounded since $V(\mathbf{x}) \to +\infty$ as $|\mathbf{x}| \to \infty$, and hence our trajectory is bounded as well. In particular, the blowup condition of Corollary A.6 can never be satisfied, and so the maximal time of existence cannot be finite. □

Even when the potential does not tend to infinity, we can still conclude global existence nearby the minima of the potential:

Corollary 1.11. *If a conservative system has a smooth potential energy $V(\mathbf{x})$ such that $V(0) = 0$, $\nabla V = 0$, and the Hessian matrix $V''(0)$ is positive definite, then there exists $r > 0$ so that solutions with initial data $(\mathbf{x}(0), \dot{\mathbf{x}}(0))$ in the ball $B_r(0)$ exist for all time.*

Proof. We follow the bootstrap argument from [Tao06].

Let $\epsilon > 0$ be a small parameter to be chosen and assume that

$$|\mathbf{x}(t)|^2 + |\dot{\mathbf{x}}(t)|^2 \leq (2\epsilon)^2 \tag{1.6}$$

for some time t. Taylor expanding about $\mathbf{x} = 0$, we have

$$V(\mathbf{x}) = \tfrac{1}{2}\mathbf{x} \cdot V''(0)\mathbf{x} + \mathcal{O}(|\mathbf{x}|^3).$$

As $V''(0)$ is positive definite and $|\mathbf{x}(t)| \leq 2\epsilon$, then we have

$$V(\mathbf{x}(t)) \geq c|\mathbf{x}(t)|^2 - C\epsilon^3$$

for some constants $c, C > 0$. By conservation of energy (Proposition 1.9), we then have

$$\tfrac{1}{2}|\dot{\mathbf{x}}(t)|^2 + c|\mathbf{x}(t)|^2 \leq E(t) + C\epsilon^3 = E(0) + C\epsilon^3$$

Picking $E(0)$ and ϵ sufficiently small, we conclude that

$$|\mathbf{x}(t)|^2 + |\dot{\mathbf{x}}(t)|^2 \leq \epsilon^2. \tag{1.7}$$

Let I denote the set of $t \in \mathbb{R}$ for which (1.7) holds. The set I is connected as $t \mapsto (\mathbf{x}(t), \dot{\mathbf{x}}(t))$ is continuous. The set I is open: we just showed that (1.6) at time t implies (1.7) for the same t, and (1.7) at time t trivially implies that (1.6) holds on a neighborhood of t. The set I is also closed, since the inequality (1.7) is a closed condition. Finally, picking r sufficiently small, we can ensure that the set I contains $t = 0$ and thus is nonempty. Altogether, the connectedness of I implies that $I = \mathbb{R}$. In particular, the blowup condition of Corollary A.6 can never be satisfied, and so the maximal time of existence cannot be finite. □

For intuition about the behavior of solutions, we can picture a small ball rolling down the graph of $V(\mathbf{x})$. Suppose we have a solution $\mathbf{x}(t)$ to Newton's equations (1.3) with $E(\mathbf{x}(t)) \equiv E_0$. As kinetic energy is nonnegative, then a ball at position $V(\mathbf{x}(t))$ is confined to the region where $V(\mathbf{x}) \leq E_0$. A smaller potential energy yields a greater kinetic energy by Proposition 1.9, which implies a greater velocity. This means that the ball gains velocity as it rolls downhill. This picture makes some facts very intuitive, like that local minima and maxima of $V(\mathbf{x})$ are stable and unstable equilibria for the system, respectively. For a general bounded region $V(\mathbf{x}) \leq E_0$, the ball rolls right through any minima and up towards the boundary $V^{-1}(E_0)$.

1.5. Linear momentum

Suppose the force on the ith particle can be decomposed as

$$\mathbf{F}_i = \sum_{\substack{j=1 \\ j \neq i}}^{N} \mathbf{F}_{ij}(t, \mathbf{x}_i, \mathbf{x}_j) + \mathbf{F}_i^{\mathrm{e}}(t, \mathbf{x}_i), \tag{1.8}$$

where $\mathbf{F}_{ij}$ is the **interaction force** between the ith and jth particle and $\mathbf{F}_i^{\mathrm{e}}$ is the **external force** on the ith particle. A system is called **closed** if there are no external forces:

$$\mathbf{F}_i^{\mathrm{e}} \equiv 0 \quad \text{for all } i.$$

We will assume that the interaction forces obey the **law of action and reaction** (or **Newton's third law**): the experimental observation that the force two particles exert on each other are equal and opposite, i.e.

$$\mathbf{F}_{ij} = -\mathbf{F}_{ji} \quad \text{for all } i, j.$$

This is a common property of Newtonian systems, and we will often be working under this assumption. If we are also given an inertial frame, then this assumption implies that the interaction forces are collinear:

$$\mathbf{F}_{ij} = f_{ij}\mathbf{e}_{ij}, \quad \text{where} \quad \mathbf{e}_{ij} = \frac{\mathbf{x}_j - \mathbf{x}_i}{|\mathbf{x}_j - \mathbf{x}_i|}.$$

Example 1.12. Any system of the form in Example 1.6 obeys the law of action and reaction since $\mathbf{e}_{ij} = -\mathbf{e}_{ji}$.

Interaction forces for non-Newtonian systems generally do not obey this law. For example, a particle with electric charge q placed in an electromagnetic field is acted upon by the Lorentz force

$$\mathbf{F} = q\left[\mathbf{E} + \tfrac{1}{c}(\mathbf{v} \times \mathbf{H})\right],$$

where $\mathbf{E}, \mathbf{H}$ are the electric and magnetic fields (which satisfy Maxwell's equations) and c is the speed of light. For a system of two electrically charged particles, the cross product term creates a non-collinear interaction force.

The effect of all external forces together can be observed through the **total (linear) momentum**

$$\mathbf{P} = \sum_{i=1}^{N} \mathbf{p}_i,$$

which is conserved for a closed system:

Proposition 1.13 (Conservation of linear momentum)**.** *The increase in total momentum is equal to the total force. Moreover, if the forces can be decomposed as* (1.8) *and satisfy the law of action and reaction, then the change in the total momentum is equal to the total external force* $\sum_i \mathbf{F}_i^{\mathrm{e}}$*. In particular, for a closed system the total linear momentum is conserved.*

Proof. By Newton's equations (1.2) we have

$$\dot{\mathbf{P}} = \sum_{i=1}^{N} \dot{\mathbf{F}}_i,$$

which is the first claim. Inserting the decomposition (1.8), we obtain

$$\dot{\mathbf{P}} = \sum_{i=1}^{N} \dot{\mathbf{p}}_i = \sum_{i=1}^{N} \mathbf{F}_i = \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \mathbf{F}_{ij} + \sum_{i=1}^{N} \mathbf{F}_i^{\mathrm{e}} = \sum_{i=1}^{N} \mathbf{F}_i^{\mathrm{e}}, \tag{1.9}$$

which is the second claim. In the last equality, we note that $\mathbf{F}_{ij} = -\mathbf{F}_{ji}$ causes the double sum over interaction forces to cancel pairwise. □

A similar argument shows that we have component-wise conservation under weaker assumptions:

Corollary 1.14. *Suppose that the forces can be decomposed as* (1.8) *and that the law of action and reaction holds. If the total external force is perpendicular to an axis, then the component of the total momentum along that axis is conserved.*

Proof. Let $\mathbf{a}$ be a unit vector so that

$$\mathbf{a} \cdot \sum_{i=1}^{N} \mathbf{F}_i^{\mathrm{e}} = 0.$$

Then taking the dot product of (1.9) with $\mathbf{a}$, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{a}\cdot\mathbf{P}) = 0$$

and thus $\mathbf{a}\cdot\mathbf{P}$ is conserved. □

As we will see later, the conservation of momentum along an axis is associated with the system's invariance under spatial translations along that axis (cf. Proposition 4.12). Specifically, we say that a system is symmetric in the direction of the unit vector $\mathbf{a}$ if whenever $\mathbf{x}_i(t)$ is a solution then so is $\mathbf{x}_i(t)+c\mathbf{a}$ for all i, for any constant c.

The total momentum can also be observed through the system's **center of mass** (or **barycenter**)

$$\mathbf{X} = \frac{\sum_{i=1}^N m_i\mathbf{x}_i}{\sum_{i=1}^N m_i}. \tag{1.10}$$

It turns out that this definition is independent of the choice or origin, and it is characterized as the point with respect to which the total momentum vanishes (cf. Exercise 1.4). Moreover, the total momentum is equivalent to all of the mass lying at the center of mass:

$$\mathbf{P} = \sum_{i=1}^N \mathbf{p}_i = M\dot{\mathbf{X}}, \qquad \text{where} \quad M = \sum_{i=1}^N m_i. \tag{1.11}$$

Proposition 1.15 (Newton's first law, general case)**.** *The center of mass evolves as if all masses were concentrated at it and all forces were applied to it. In particular, for a closed system the motion of the center of mass is rectilinear (i.e. uniform in time with constant velocity).*

Proof. Differentiating (1.11) yields

$$M\ddot{\mathbf{X}} = \dot{\mathbf{P}} = \sum_{i=1}^n \mathbf{F}_i.$$

The RHS vanishes for a closed system by (1.9). □

1.6. Angular momentum

In this section, we will specialize to the case $d = 3$ so that we may use the cross product on $\mathbb{R}^3$. The **angular momentum** (about the origin) of the ith particle and the **total angular momentum** are given by

$$\mathbf{L}_i = \mathbf{x}_i \times \mathbf{p}_i, \qquad \mathbf{L} = \sum_{i=1}^N \mathbf{L}_i$$

respectively. The **torque** (or **moment of force**) of the ith particle and the **total torque** are given by

$$\mathbf{N}_i = \mathbf{x}_i \times \mathbf{F}_i, \qquad \mathbf{N} = \sum_{i=1}^{N} \mathbf{N}_i$$

respectively.

When the forces can be decomposed as (1.8), we define the **external torque**

$$\mathbf{N}_i^{\mathrm{e}} = \mathbf{x}_i \times \mathbf{F}_i^{\mathrm{e}}.$$

The relationship between angular momentum and torque is analogous to their linear counterparts:

Proposition 1.16 (Conservation of angular momentum)**.** *The increase in total angular momentum is equal to the total torque. Moreover, if the forces can be decomposed as* (1.8) *and satisfy the law of action and reaction, then the change in total angular momentum is equal to the total external torque* $\sum_i \mathbf{N}_i^{\mathrm{e}}$*. In particular, for a closed system the total angular momentum is conserved.*

Proof. By Newton's equations (1.2) we have

$$\dot{\mathbf{L}} = \sum_{i=1}^{N} \dot{\mathbf{L}}_i = \sum_{i=1}^{N} \left(\mathbf{x}_i \times \dot{\mathbf{p}}_i + \dot{\mathbf{x}}_i \times \mathbf{p}_i \right) = \sum_{i=1}^{N} \mathbf{x}_i \times \mathbf{F}_i + 0 = \mathbf{N},$$

which is the first claim. In the third equality we noted that the term $\dot{\mathbf{x}}_i \times \mathbf{p}_i$ vanishes because $\mathbf{p}_i$ is parallel to $\dot{\mathbf{x}}_i$. Assuming the decomposition (1.8), we obtain

$$\dot{\mathbf{L}} = \sum_{i=1}^{N} \mathbf{x}_i \times \mathbf{F}_i = \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \mathbf{x}_i \times \mathbf{F}_{ij} + \sum_{i=1}^{N} \mathbf{x}_i \times \mathbf{F}_i^{\mathrm{e}} = \sum_{i=1}^{N} \mathbf{N}_i^{\mathrm{e}}, \tag{1.12}$$

which is the second claim. In the last equality we noted that $\mathbf{F}_{ij} = -\mathbf{F}_{ji}$ causes the double sum cancels pairwise:

$$\mathbf{x}_i \times \mathbf{F}_{ij} + \mathbf{x}_j \times \mathbf{F}_{ji} = (\mathbf{x}_i - \mathbf{x}_j) \times \mathbf{F}_{ij} = 0.$$

In particular, for a closed system the RHS of (1.12) vanishes and we have $\dot{\mathbf{L}} = 0$. □

A similar argument shows that we have component-wise conservation under weaker assumptions:

Corollary 1.17. *Suppose that the forces can be decomposed as* (1.8) *and that the law of action and reaction holds. If the total external torque is perpendicular to an axis, then the projection of the total angular momentum onto that axis is conserved.*

Proof. Let $\mathbf{a}$ be a unit vector so that

$$\mathbf{a} \cdot \sum_{i=1}^{N} \mathbf{N}_i^{\mathrm{e}} = 0.$$

Then taking the dot product of (1.9) with $\mathbf{a}$, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{a} \cdot \mathbf{L}) = 0$$

and thus $\mathbf{a} \cdot \mathbf{L}$ is conserved. □

As we will see later, the conservation of angular momentum about an axis is associated with invariance under rotations about that axis (cf. Proposition 4.12). Specifically, we say that the system is rotationally symmetric about the unit vector $\mathbf{a}$ if whenever $\mathbf{x}_i(t)$ is a solution then so is $\mathbf{x}_i(t)\cos\theta + \mathbf{a} \times \mathbf{x}_i(t)\sin\theta + \mathbf{a}(\mathbf{a} \cdot \mathbf{x}_i(t))(1 - \cos\theta)$ for all i, for any constant θ.

The center of mass also plays an important role for angular momentum. Indeed, the total angular momentum evolves as if it were all concentrated at the center of mass and all the external torques were applied to it:

Proposition 1.18. *The total angular momentum (or total torque) about the origin is equal to the sum of the total angular momentum (total torque) about the center of mass and the angular momentum (torque) of the center of mass about the origin.*

Proof. Expanding about the center of mass, we have

$$\begin{aligned}
\mathbf{L} &= \sum_{i=1}^{N} [(\mathbf{x}_i - \mathbf{X}) + \mathbf{X}] \times m_i \big[(\dot{\mathbf{x}}_i - \dot{\mathbf{X}}) + \dot{\mathbf{X}}\big] \\
&= \sum_{i=1}^{N} (\mathbf{x}_i - \mathbf{X}) \times m_i(\dot{\mathbf{x}}_i - \dot{\mathbf{X}}) + \mathbf{X} \times M\dot{\mathbf{X}} \\
&\quad + \left[\sum_{i=1}^{N} m_i(\mathbf{x}_i - \mathbf{X})\right] \times \dot{\mathbf{X}} + \mathbf{X} \times \left[\sum_{i=1}^{N} m_i(\dot{\mathbf{x}}_i - \dot{\mathbf{X}})\right] \\
&= \sum_{i=1}^{N} (\mathbf{x}_i - \mathbf{X}) \times m_i(\dot{\mathbf{x}}_i - \dot{\mathbf{X}}) + \mathbf{X} \times \mathbf{P} + 0 + 0
\end{aligned}$$

which yields the claim for angular momentum. In the last equality we used the definition of total momentum (1.11) for the first term and Exercise 1.4 for the vanishing of the square-bracketed terms. The statement for torque follows by taking a time derivative. □

There is one more dynamical quantity of interest: the **moment of inertia** of the ith particle (about the origin), which is given by

$$I_i = m_i|\mathbf{x}_i|^2.$$

The moment of inertia plays a role for the **angular velocity**

$$\boldsymbol{\omega}_i = \frac{\mathbf{x}_i \times \dot{\mathbf{x}}_i}{|\mathbf{x}_i|^2}$$

analogous to that of mass for linear velocity, in the sense that

$$\mathbf{L}_i = \mathbf{x}_i \times \mathbf{p}_i = \mathbf{x}_i \times (m_i \boldsymbol{\omega}_i \times \mathbf{x}_i) = m_i \left[(\mathbf{x}_i \cdot \mathbf{x}_i)\boldsymbol{\omega}_i - (\mathbf{x}_i \cdot \boldsymbol{\omega}_i)\mathbf{x}_i \right] = I_i \boldsymbol{\omega}_i + 0.$$

As in the previous proposition, the formula $\mathbf{L} = I\boldsymbol{\omega}$ can also be translated to the center of mass.

Unlike mass, the moment of inertia evolves in time:

Proposition 1.19. *The total moment of inertia evolves according to*

$$\ddot{I} = 4K + 2\mathbf{F} \cdot \mathbf{x}. \tag{1.13}$$

In particular, for a conservative system with homogeneous potential $V(\mathbf{x}) = c|\mathbf{x}|^k$ *we have*

$$\ddot{I} = 4E - 2(k+2)V. \tag{1.14}$$

Proof. The first claim (1.13) is a straightforward calculation. For the second claim (1.14), we note that for a homogeneous potential we have

$$\mathbf{F} \cdot \mathbf{x} = -\nabla V \cdot \mathbf{x} = -kV, \qquad 4K = 4E - 4V. \qquad \square$$

1.7. Exercises

1.1 (Galilean group generators)**.** Show that every Galilean transformation g on $\mathbb{R} \times \mathbb{R}^d$ can be uniquely written as the composition $g_1 \circ g_2 \circ g_3$ of the three types of Galilean transformations in Example 1.2. What is the dimension of the group of Galilean transformations for $d = 3$? (Hint: Start by writing g as the general affine transformation

$$g(t, \mathbf{x}) = (\mathbf{b} \cdot \mathbf{x} + kt + t_0, A\mathbf{x} + \mathbf{v}t + \mathbf{x}_0),$$

and show that $\mathbf{b} = 0$, $k = 1$, and $A \in O(d)$.)

1.2. Suppose a Newtonian system of N particles in $\mathbb{R}^d$ is in an inertial frame and all of the initial velocities are zero. Show that if the particles are initially contained in a $(d-1)$-dimensional linear subspace of $\mathbb{R}^d$ then they remain in that subspace for all time.

1.3 (Rotating reference frame)**.** Suppose we have a system in an inertial coordinate frame $\mathbf{z} \in \mathbb{R}^3$ (e.g. coordinates relative to the sun), so that Newton's equations (1.3) obey the conditions (a)–(c) of section 1.1. Consider another set of non-inertial coordinates $\mathbf{x}$ (e.g. coordinates relative to a point on Earth's surface) expressed in terms of the coordinates $\mathbf{z}$ via

$$t \mapsto t, \qquad \mathbf{z} \mapsto \mathbf{x} = B(t)\mathbf{z} + \mathbf{b}(t).$$

Here, $\mathbf{b}(t) \in \mathbb{R}^3$ is the new origin and $B(t) \in O(3)$ is a rotation matrix for all t.

(a) Show that the equations of motion in the new frame are

$$m_i\ddot{\mathbf{z}}_i = \mathbf{F}_i\big(\mathbf{z}_k - \mathbf{z}_j, B^{-1}\dot{B}(\mathbf{z}_k - \mathbf{z}_j) + (\dot{\mathbf{z}}_k - \dot{\mathbf{z}}_j)\big) + \mathbf{\Phi}_i + \mathbf{\Psi}_i,$$

where

$$\mathbf{\Phi}_i = -m_i\big(B^{-1}\ddot{B}\mathbf{z}_i + B^{-1}\ddot{\mathbf{b}}\big), \qquad \mathbf{\Psi}_i = -2m_iB^{-1}\dot{B}\dot{\mathbf{z}}_i.$$

The new forces $\mathbf{\Phi}_i$ and $\mathbf{\Psi}_i$ that appear in the equations of motion for $\mathbf{z}$ are called **inertial** or **fictitious forces**.

(b) Differentiate the definition of an orthogonal matrix to show that $B^{-1}\dot{B}$ is antisymmetric, and write $B^{-1}\dot{B}\mathbf{z} = \boldsymbol{\omega} \times \mathbf{z}$ where $\boldsymbol{\omega}$ is the angular velocity of the moving frame. Now we have

$$\mathbf{\Psi}_i = -2m_i\boldsymbol{\omega} \times \dot{\mathbf{z}}.$$

$\mathbf{\Psi}_i$ is called the **Coriolis force**, and depends on the velocity. In the northern hemisphere on Earth, it deflects every moving body to the right and every falling body to the east.

(c) Let $\mathbf{w} = B^{-1}\mathbf{b}$ denote the **acceleration** and $\boldsymbol{\alpha} = \dot{\boldsymbol{\omega}}$ denote the **angular acceleration** of the moving frame. Use the time derivative of $B^{-1}\dot{B}$ to show that

$$\mathbf{\Phi}_i = -m_i\big[\mathbf{w} + \boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{z}_i) + \boldsymbol{\alpha} \times \mathbf{z}_i\big].$$

The second term is called the **centrifugal force** and the third term is the **inertial rotation force** or the **Euler force**, both of which only depend on position. The former is always directed outward from the instantaneous axis of rotation and acts even on a body at rest in the coordinate system $\mathbf{z}$. The latter is only present for nonuniform rotation.

1.4 (Center of mass)**.** (a) Show that the center of mass (1.10) does not depend on the choice of origin.

(b) Show that both the "total position" and total momentum relative to the center of mass vanishes:

$$\sum_{i=1}^{N} m_i(\mathbf{x}_i - \mathbf{X}) = 0, \qquad \sum_{i=1}^{N} m_i(\dot{\mathbf{x}}_i - \dot{\mathbf{X}}) = 0.$$

1.5 (A way to compute π [Gal03])**.** In this example we will see a geometric aspect of phase space appear as a physically measurable quantity. This reinforces that phase space is an inherent object of a Newtonian system and not merely an abstract concept.

Consider a frictionless horizontal ray with a vertical wall at the origin. One small block of mass m is initially at rest on the surface, and a big block of mass $M \gg m$ is pushed towards the small block so that the small block is sandwiched between the large block and the wall. We will count the number of collisions N the small block makes with the big block or the wall.

(a) Let v_1 and v_2 denote the velocities of the large and small blocks respectively, and consider the rescaling $y_1 = \sqrt{M}v_1$, $y_2 = \sqrt{m}v_2$. Plot the initial energy level set in the (y_1, y_2)-plane to which the motion is confined.

(b) Initially we have $v_1 < 0$, $v_2 = 0$; plot this point in the same (y_1, y_2)-plane. Assume that each collision is **purely elastic**, so that when the blocks collide the total momentum is conserved. Plot the total momentum level set which contains the initial point; the outcome velocities is determined by the other intersection of the level sets. After the first collision the small block will eventually hit the wall, and we will assume that this collision is also elastic so that $v_2 < 0$ is replaced by $-v_2 > 0$; plot this new point as well. Plot a few more iterates of this two-collision pattern in the (y_1, y_2)-plane.

(c) The pattern repeats until $v_1 > 0$ and $0 < v_2 < v_1$, so that the large block is moving away and the small block will neither collide with the wall again nor catch up to the large block. Sketch this final configuration region in the (y_1, y_2)-plane.

(d) Connect consecutive points occupied by the system in the (y_1, y_2)-plane. As the lines are either vertical or parallel, the angle θ at a point between any two consecutive lines is the same. Show that $\theta = \arctan\sqrt{m/M}$.

(e) For any point, the angle θ at that point subtends an arc on the circle opposite that point. By considering the length of this arc, show that the total number N of collisions that occurs is the largest integer such that $N\theta < \pi$.

(f) Take $M = 100^n m$ for $n > 0$ an integer. Show that $10^{-n}N \to \pi$ as $n \to \infty$, and so the number N of collisions spells out the digits of π for n sufficiently large.

1.6 (Book stacking [Nah16])**.** We will stack books of mass 1 and length 1 on a table in an effort to produce the maximum amount of overhang.

(a) Place the first book with its left edge at $x = 0$ and its right edge lined up with the end of the table at $x = 1$. By considering the center of mass of the book, determine the distance $S(1)$ we can slide the book over the edge of the table before it falls.

(b) Starting with a stack of two books, we can reason as in part (a) and slide the top book forward a distance of $S(1)$ while keeping the bottom book stationary. By considering the center of mass of the two books, determine the distance $S(2)$ we can slide this two-book configuration before it falls.

(c) Now start with three books, slide the top one a distance of $S(1)$ and then the top two books as in part (b) in order to produce an overhang $S(2)$ from the edge of the bottom book. Determine the distance $S(3)$ we can slide the three-book configuration before it falls.

(d) Postulate a formula for $S(n)$ and prove it by induction. Note that the overhang $S(n)$ tends to infinity as $n \to \infty$.

1.7. Consider a conservative system in $\mathbb{R}^3$ with coordinates so that the center of mass $\mathbf{X} = 0$ is at the origin and is at rest, i.e. $\dot{\mathbf{X}} = 0$.

(a) Show that $|\mathbf{L}|^2 \leq 2IK$.

(b) Show that the trajectories in configuration space must be contained in the intersection of the hyperplane $\{\mathbf{x} \in \mathbb{R}^{3N} : \sum_{i=1}^{N} m_i \mathbf{x}_i = 0\}$ with the set $\{\mathbf{x} \in \mathbb{R}^{3N} : V(\mathbf{x}) + |\mathbf{L}|^2/(2I(\mathbf{x})) \leq E\}$, where $\mathbf{L}$ and E are constant in time.

CHAPTER 2

ONE DEGREE OF FREEDOM

As Newton's equations model a mechanical system, they come with some special structure. In this chapter, we will see some of the implications that this has for solutions. Although many of the definitions extend to arbitrary dimensions, we will focus on the case of one degree of freedom where the consequences are particularly clear (because trajectories in phase space have codimension one). Sections 2.1 to 2.4 are based on [Str15, Ch. 5–7] and [JS07, Ch. 10], and section 2.5 is based on [LL76, Ch. 3] and [Arn89, Ch. 2].

2.1. Linear systems

Suppose we have a Newtonian system with one degree of freedom, and that the force is only a function of position:

$$m\ddot{x} = F(x).$$

Any such system is automatically conservative, because we can always find an antiderivative $-V(x)$ (unique up to an additive constant) so that

$$m\ddot{x} = -V'(x). \tag{2.1}$$

We want to understand the qualitative behavior of solutions near a given point x_0. We may assume that $x_0 = 0$ for convenience, after replacing the variable x by $x - x_0$ if necessary.

First we begin with the generic case $V'(0) \neq 0$. In phase space $\mathbb{R}_x \times \mathbb{R}_p$, this means that the vector field $(\dot{x}, \dot{p})$ at the origin is nonzero. From the general theory of ODEs (cf. Proposition A.18), this implies that there is a smooth change of variables in a neighborhood of the origin so that the vector field is constant. More specifically, we have $\dot{p} \approx -V'(0)$ near the origin, and so the solution $x(t)$ is accelerating to the left if $V'(0) > 0$ and to the right if $V'(0) < 0$.

With this easy case out of the way, we will now assume $V'(0) = 0$ for the remainder of this section. The point $(x_0, p_0) = (0, 0)$ is then a **fixed point** (or **equilibrium**) of the flow, meaning that the constant function $x(t) \equiv 0$ (and $p(t) \equiv 0$) solves the equation. Our first step is to linearize: Taylor expanding about $x = 0$ and keeping only the linear term, we obtain

$$m\ddot{x} = -V'(x) \approx -V'(0) - V''(0)x = -V''(0)x. \tag{2.2}$$

The behavior of solutions to this approximate equation depends on the sign of $V''(0)$.

We begin with the case $V''(0) < 0$:

Example 2.1 (Saddle node)**.** Consider the linear system

$$m\ddot{x} = kx$$

for $k > 0$ a constant. This is a conservative system with potential and total energy

$$V(x) = -\tfrac{1}{2}kx^2, \qquad E(x,p) = \tfrac{1}{2m}p^2 - \tfrac{1}{2}kx^2.$$

The trajectories in phase space are confined to the level sets of E, which look like axes-symmetric hyperbolas. The origin is a **saddle node** for this linear system, and we have the explicit solutions

$$x(t) = x_0 \cosh(\gamma t) + \tfrac{p_0}{m\gamma}\sinh(\gamma t), \qquad p(t) = m\gamma x_0 \sinh(\gamma t) + p_0 \cosh(\gamma t),$$

where $\gamma = \sqrt{\frac{k}{m}}$.

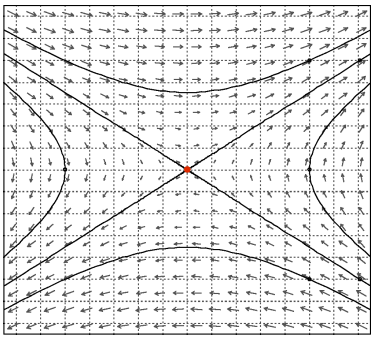


Figure 2.1: Phase portrait for the system of Example 2.1.

We would like to know if the solutions to the approximate equation (2.2) provide an accurate prediction for the solutions to the actual equation (2.1). From ODE theory, the Hartman–Grobman theorem (Theorem A.21) tells us that there is a continuous change of variables from the nonlinear system to the linearized system, provided that all the eigenvalues of the linearized system have nonzero real parts. The theorem applies in this case, because we have the matrix

$$\begin{pmatrix} \dot{x} \\ \dot{p} \end{pmatrix} = \begin{bmatrix} 0 & \frac{1}{m} \\ k & 0 \end{bmatrix} \begin{pmatrix} x \\ p \end{pmatrix}$$

with eigenvalues $\pm\sqrt{\frac{k}{m}}$.

Next we consider the case $V''(0) > 0$:

Example 2.2 (Harmonic oscillator)**.** Consider the linear system

$$m\ddot{x} = -kx$$

for $k > 0$ a constant. This is a conservative system with potential and total energy

$$V(x) = \tfrac{1}{2}kx^2, \qquad E(x,p) = \tfrac{1}{2m}p^2 + \tfrac{1}{2}kx^2.$$

The trajectories in phase space are confined to the level sets of E, which look like axes-parallel ellipses centered at the origin. The origin is called a **center** for this linear system, and we have the explicit solutions

$$x(t) = x_0\cos(\omega t) + \tfrac{p_0}{m\omega}\sin(\omega t), \qquad p(t) = -m\omega x_0\sin(\omega t) + p_0\cos(\omega t),$$

where $\omega = \sqrt{\frac{k}{m}}$.

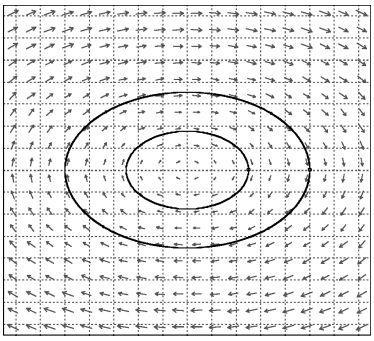


Figure 2.2: Phase portrait for the system of Example 2.2.

Unfortunately, we are unable to immediately conclude that this is an accurate description of the actual equation (2.1) because the Hartman–Grobman theorem no longer applies. Indeed, our matrix is

$$\begin{pmatrix}\dot{x}\\ \dot{p}\end{pmatrix} = \begin{bmatrix}0 & \frac{1}{m}\\ -k & 0\end{bmatrix}\begin{pmatrix}x\\ p\end{pmatrix}$$

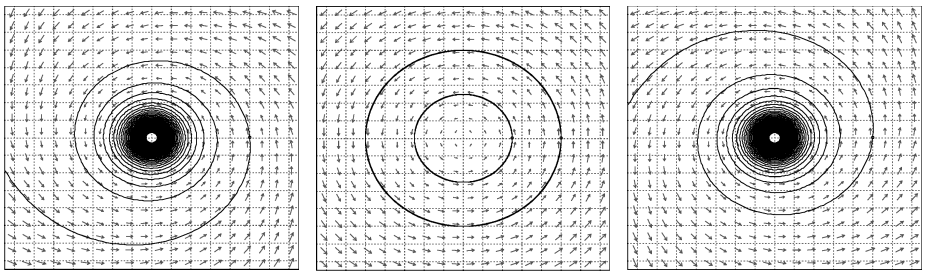
with purely imaginary eigenvalues $\pm i\sqrt{\frac{k}{m}}$.

We might hope that the conclusion of the Hartman–Grobman theorem still persists. This is not obvious however, because the premise of the theorem is necessary as the following example illustrates:

Example 2.3. Consider the system

$$\begin{array}{c}\dot{x} = -y + ax(x^2+y^2)\\ \dot{y} = x + ay(x^2+y^2)\end{array} \quad\Longleftrightarrow\quad \begin{array}{c}\dot{r} = ar^3\\ \dot{\theta} = 1\end{array}$$

on $\mathbb{R}^2$, where $a \in \mathbb{R}$ is a constant. When $a = 0$ we obtain the linearized system at $(x_*, y_*) = (0, 0)$, which has eigenvalues $\pm i$ and predicts that the origin is a center. However, when $a < 0$ ($a > 0$) we see that $r(t)$ is decreasing (increasing) monotonically and so the origin becomes a stable (unstable) spiral.



(a) $a < 0$ (b) $a = 0$ (c) $a > 0$

Figure 2.4: Phase portraits for the system of Example 2.3.

We will see in sections 2.2 and 2.4 that the prediction of Example 2.2 is indeed accurate for conservative systems, because the mechanical system (2.1) has special properties in comparison to general ODEs.

Finally, consider the case $V''(0) = 0$. Then the equation $m\ddot{x} = 0$ can be directly integrated to obtain a linear function for $x(t)$, which describes rectilinear motion (uniform motion with constant velocity). This is of course not a robust prediction since $\dot{p}$ is nonzero whenever $V' \neq 0$, and so we cannot draw any conclusions.

2.2. Conservative systems

In section 1.4 we saw that for a conservative Newtonian system the total mechanical energy is constant along trajectories. We will now give this mathematical phenomenon a name and examine its consequences. In addition to conservative mechanical systems, this also applies to some systems of ODEs which do not arise from mechanics (cf. Exercise 2.2).

Suppose we have the first-order ODE system

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) \tag{2.3}$$

defined for $\mathbf{x}$ in an open set $U \subset \mathbb{R}^n$. We can always reduce a degree-d system of ODEs to such a first-order system (at the cost of increasing the dimension) by treating the time derivatives $\dot{\mathbf{x}}, \ddot{\mathbf{x}}, \ldots, \mathbf{x}^{(d-1)}$ as new independent variables.

Definition 2.4. A **conserved quantity** for the ODE system (2.3) is a smooth function $E : U \to \mathbb{R}$ that is nonconstant on open subsets of U and satisfies $\frac{\mathrm{d}}{\mathrm{d}t}(E(\mathbf{x}(t))) = 0$ for all solutions $\mathbf{x}(t)$ to (2.3).

Geometrically, this requires that solutions $\mathbf{x}(t)$ lie in level sets of $E(\mathbf{x})$, and so the quantity E restricts the directions in which trajectories may travel. We require that E is nonconstant on open sets so that E rules out some directions. For example, the constant function $E(\mathbf{x}) \equiv 10$ is trivially conserved, but it does not reveal any information about the behavior of solutions.

A point $\mathbf{x}_*$ where $\mathbf{f}(\mathbf{x}_*) = 0$ is called a **fixed point** (or **equilibrium**) of (2.3). This implies that the constant function $\mathbf{x}(t) \equiv \mathbf{x}_*$ is a solution of (2.3).

A fixed point $\mathbf{x}_*$ is **attracting** if there exists an open ball $B_\epsilon(\mathbf{x}_*)$ centered at $\mathbf{x}_*$ so that for any initial condition $\mathbf{x}(0) \in B_\epsilon(\mathbf{x}_*)$ the corresponding solutions $\mathbf{x}(t)$ converge to $\mathbf{x}_*$ as $t \to \infty$. Likewise, a fixed point $\mathbf{x}_*$ is **repulsive** if the same statement holds with $-t$ in place of t.

Proposition 2.5. *If the ODE system* (2.3) *has a conserved quantity, then there are no attracting (or repulsive) fixed points.*

Proof. Suppose $\mathbf{x}_*$ were an attracting fixed point, and let $\epsilon > 0$ such that $\mathbf{x}(t) \to \mathbf{x}_*$ as $t \to \infty$ for all initial conditions $\mathbf{x}(0) \in B_\epsilon(\mathbf{x}_*)$. Using that E is continuous and is constant on the trajectory $\mathbf{x}(t)$, we have

$$E(\mathbf{x}(0)) = \lim_{t\to\infty} E(\mathbf{x}(t)) = E(\mathbf{x}_*).$$

As $\mathbf{x}(0) \in B_\epsilon(\mathbf{x}_*)$ was arbitrary we conclude that E is constant on the open ball $B_\epsilon(\mathbf{x}_*)$, which contradicts our definition of a conserved quantity

Substituting $t \mapsto -t$ yields the claim for repulsive fixed points. □

In order to understand the qualitative behavior of solutions near a fixed point $\mathbf{x}_*$, we can try to linearize about $\mathbf{x}_*$ as in section 2.1:

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) \approx \mathbf{f}(\mathbf{x}_*) + D\mathbf{f}(\mathbf{x}_*)(\mathbf{x} - \mathbf{x}_*) = D\mathbf{f}(\mathbf{x}_*)(\mathbf{x} - \mathbf{x}_*), \tag{2.4}$$

where $D\mathbf{f}(\mathbf{x}_*)$ is the derivative matrix of $\mathbf{f}$ at $\mathbf{x}_*$. Recall from Example 2.3 that when the linearized system predicts that $\mathbf{x}_*$ a center, we cannot conclude that solutions to the nonlinear system (2.3) form closed orbits (i.e. periodic trajectories). This is because centers are delicate in the sense that trajectories need to perfectly match up after one revolution, and the neglected terms in the Taylor expansion (2.4) can prevent this by pushing them slightly inwards or outwards.

In two dimensions, the presence of a conserved quantity is enough to recover the prediction:

Theorem 2.6 (Nonlinear centers for conservative systems)**.** *Suppose the two-dimensional ODE system* (2.3) *has an isolated fixed point* $\mathbf{x}_*$ *and that* $E(\mathbf{x})$ *is a conserved quantity. If* $\mathbf{x}_*$ *is an isolated critical point of* E *and the Hessian matrix* $E''(\mathbf{x}_*)$ *is positive (or negative) definite, then all trajectories sufficiently close to* $\mathbf{x}_*$ *are closed.*

Proof. We will consider the case where $\mathbf{x}_*$ is a minimum of E. Replacing E by $-E$ then yields the claim for a maximum of E.

Fix $\epsilon > 0$ sufficiently small so that $\mathbf{x}_*$ is the only fixed point of $\mathbf{f}$ in $B_\epsilon(\mathbf{x}_*)$, $\mathbf{x}_*$ is the only critical point of E in $B_\epsilon(\mathbf{x}_*)$, and $E''(\mathbf{x})$ is positive definite on $B_\epsilon(\mathbf{x}_*)$.

Fix $\mathbf{x}_0 \in B_\epsilon(\mathbf{x}_*) \setminus \{\mathbf{x}_*\}$. Let $c = E(\mathbf{x}_0)$, and consider the component γ of the level set $E^{-1}(c)$ in $B_\epsilon(\mathbf{x}_*)$ containing $\mathbf{x}_0$. We claim that γ is a simple closed contour containing $\mathbf{x}_*$. For each $\theta \in [0, 2\pi)$, consider the value $r(\theta) > 0$ such that

$$E(r(\theta)\cos\theta, r(\theta)\sin\theta) = c.$$

As $\mathbf{x}_*$ is a strict local minimum of E, then we may take ϵ smaller if necessary to ensure that $r(\theta)$ exists for all θ. The choice of $r(\theta)$ is then unique since E is strictly convex on $B_\epsilon(\mathbf{x}_*)$. The function $\theta \mapsto (r(\theta)\cos\theta, r(\theta)\sin\theta)$ now provides a continuous parameterization of γ, and thus γ is a simple closed contour containing $\mathbf{x}_*$. In fact, we know that γ is also smooth by the implicit function theorem since ∇E is nonzero on γ.

Next, we claim that the trajectory $\mathbf{x}(t)$ starting at $\mathbf{x}_0$ must be periodic. We know that $\mathbf{x}(t)$ exists for all $t \in \mathbb{R}$, because it is confined to the bounded set γ and so the blowup condition of Corollary A.6 can never be satisfied. Suppose for a contradiction that $\mathbf{x}(t)$ never repeats any value. Consider the sequence $\mathbf{x}(1), \mathbf{x}(2), \ldots$. It is contained in the closed and bounded set γ, and thus must admit a convergent subsequence. Along this sequence the derivative $\dot{\mathbf{x}} = \mathbf{f}$ is converging to zero. As $\mathbf{f}$ is continuous then the value of $\mathbf{f}$ at the limit point must be zero, which contradicts that γ does not contain a fixed point. Moreover, $\mathbf{x}(t)$ must hit every point on γ since there are no fixed points on γ and γ is connected.

Therefore the trajectory starting at $\mathbf{x}_0$ is periodic. As $\mathbf{x}_0 \in B_\epsilon(\mathbf{x}_*) \setminus \{\mathbf{x}_*\}$ was arbitrary, we conclude that all trajectories in $B_\epsilon(\mathbf{x}_*) \setminus \{\mathbf{x}_*\}$ are closed orbits. □

In Theorem 2.6 we must assume that $\mathbf{x}_*$ is an isolated fixed point, otherwise there could be fixed points on the energy contour (cf. Exercise 2.3).

2.3. Nonconservative systems

In practice, we know that mechanical systems are never exactly conservative: dissipative forces (e.g. kinetic friction) dampen the motion and prevent trajectories from being perfectly periodic. However, we still have $\frac{\mathrm{d}}{\mathrm{d}t}E \leq 0$ in this case, which has new mathematical consequences for solutions.

Definition 2.7. Consider the first-order ODE system (2.3) with a fixed point $\mathbf{x}_*$. Suppose there exists a smooth function $E(\mathbf{x})$ on a connected neighborhood U of the fixed point $\mathbf{x}_*$ such that $\mathbf{x}_*$ is a strict global minimum with value zero, and for all $c > 0$ the sub-level sets $\{\mathbf{x} : E(\mathbf{x}) \leq c\}$ within U are compact and star-shaped about $\mathbf{x}_*$ with smooth boundary. If also:

(a) $\frac{\mathrm{d}}{\mathrm{d}t}E(\mathbf{x}) \leq 0$ for all $\mathbf{x}$ in $U \setminus \{\mathbf{x}_*\}$, then E is a (**weak**) **Lyapunov function**.

(b) $\frac{\mathrm{d}}{\mathrm{d}t}E(\mathbf{x}) < 0$ for all $\mathbf{x}$ in $U \setminus \{\mathbf{x}_*\}$, then E is a **strong Lyapunov function**.

The star-shaped assumption clearly guarantees that the level sets of E near $\mathbf{x}_*$ have an interior and exterior. While there do exist topological results that we could rely upon to weaken this hypothesis (cf. the Jordan curve theorem and its extensions), Definition 2.7 is suitable for our purposes and is easily verified in practice. In particular, the star-shaped criterion is satisfied if E'' is positive definite, as we will now show. However, note that our definition can also allow for higher-order minima on a case-by-case basis.

Lemma 2.8. *If $E : U \to \mathbb{R}$ is smooth on an open set $U \subset \mathbb{R}^n$, $\mathbf{x}_* \in U$ is an isolated critical point of E with $E(\mathbf{x}_*) = 0$, and the Hessian matrix $E''(\mathbf{x}_*)$ is positive definite, then there exists $\epsilon > 0$ sufficiently small so that the sub-level sets $\{\mathbf{x} \in B_\epsilon(\mathbf{x}) : E(\mathbf{x}) \leq c\}$ for $c \in E(B_\epsilon(\mathbf{x}_*))$ are compact and star-shaped about $\mathbf{x}_*$ with smooth boundary.*

Proof. Fix $\epsilon > 0$ sufficiently small so that $\mathbf{x}_*$ is the only critical point of E in $B_\epsilon(\mathbf{x}_*)$ and $E''(\mathbf{x})$ is positive definite on $B_\epsilon(\mathbf{x}_*)$. For each unit vector $\nu \in \mathbb{R}^n$, $|\nu| = 1$ consider the value $r(\nu) > 0$ such that

$$E(r(\nu)\nu) = c.$$

As $\mathbf{x}_*$ is a strict local minimum of E, then we may take ϵ smaller if necessary to ensure that $r(\nu)$ exists for every $|\nu| = 1$. The choice of $r(\nu)$ is then unique since E is strictly convex. Finally, $r(\nu)$ is smooth since ∇E is nonvanishing on the level set $E(\mathbf{x}) = c$. □

A physical example of a Lyapunov function is the total energy of a dissipative system:

Example 2.9 (Damped harmonic oscillator)**.** Consider the system

$$m\ddot{x} = -b\dot{x} - kx$$

with one degree of freedom, where $b > 0$ a damping constant. The total energy is still

$$E = \tfrac{1}{2}(m\dot{x}^2 + kx^2),$$

but now

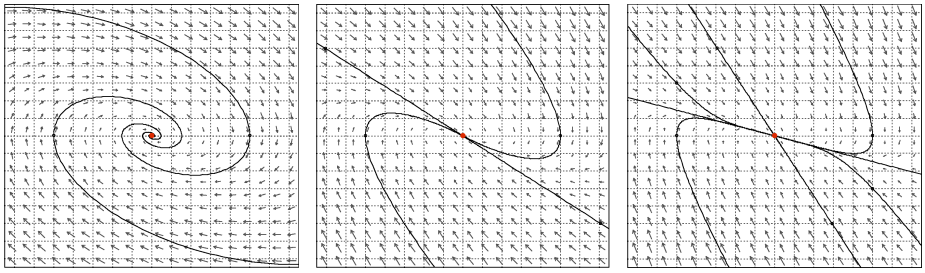
$$\frac{\mathrm{d}}{\mathrm{d}t}E = m\dot{x}\ddot{x} + kx\dot{x} = -b\dot{x}^2 \leq 0.$$

The total energy E is a weak (but not strong) Lyapunov function. The origin is globally attracting with three qualitatively different phase portraits:

(a) $0 < b < 2\sqrt{km}$: **Under damped**. The origin is a stable spiral node and the system oscillates infinitely many times with exponentially decaying amplitude.

(b) $b = 2\sqrt{km}$: **Critically damped**. The origin is a stable degenerate node. The oscillation and friction balance each other so that trajectories barely fail to make one complete oscillation. In fact, trajectories approach the origin faster than in the other two cases.

(c) $b > 2\sqrt{km}$: **Over damped**. The origin is a stable node and the system returns to the origin without oscillating.



(a) Under damped (b) Critically damped (c) Over damped

Figure 2.6: Phase portraits for the system of Example 2.9.

For our image of the ball rolling down the graph of the potential energy, the surface of the graph is now slightly sticky. The ball may still roll through a minimum, but does not have enough energy to approach the boundary $V^{-1}(E_0)$ again and so the permitted region for the ball continually shrinks. If V is shaped like a bowl about $\mathbf{x}_*$ as in the definition of a Lyapunov function, then we intuitively expect that the ball tends to the bottom of the bowl and hence $\mathbf{x}_*$ is stable.

Theorem 2.10. *Consider the smooth n-dimensional ODE system* (2.3) *with a fixed point $\mathbf{x}_*$.*

(a) If there exists a weak Lyapunov function on a neighborhood of the fixed point $\mathbf{x}_*$, then $\mathbf{x}_*$ is Lyapunov stable: for any $\epsilon > 0$ there exists $\delta > 0$ such that $|\mathbf{x}(0) - \mathbf{x}_*| < \delta$ implies $|\mathbf{x}(t) - \mathbf{x}_*| < \epsilon$ for all $t \geq 0$.

(b) If $n = 2$ and there exists a strong Lyapunov function near the fixed point $\mathbf{x}_*$, then $\mathbf{x}_*$ is also asymptotically stable: there exists $\eta > 0$ so that $|\mathbf{x}(0) - \mathbf{x}_*| < \eta$ implies $\mathbf{x}(t) \to \mathbf{x}_*$ as $t \to \infty$.

In particular, if there exists a strong Lyapunov function then there can be no periodic solutions, unlike conservative systems.

In part (a) of Theorem 2.10, we cannot expect the fixed point to by asymptotically stable in general: for the harmonic oscillator (Example 2.2) the total energy is conserved and thus serves as a weak Lyapunov function. On the other hand, all cases of the damped harmonic oscillator (Example 2.9) only possess a weak Lyapunov function and yet they still enjoy the additional conclusion of part (b). This happens because no trajectory can remain in the set where $\frac{\mathrm{d}}{\mathrm{d}t}E(\mathbf{x}) = 0$. In fact, for such systems the conclusion of case (b) can be recovered under additional assumptions; see [JS07, §10.5] for details.

Proof. (a) Fix $\epsilon > 0$. After shrinking ϵ if necessary, we may assume $B_\epsilon(\mathbf{x}_*) \subset U$. As $\mathbf{x}_*$ is a strict local minimum of E, there exists $c > 0$ sufficiently small so that the sub-level set $\{E(\mathbf{x}) \leq c\}$ is contained in $B_\epsilon(\mathbf{x}_*)$. Pick $\delta > 0$ so that the ball $B_\delta(\mathbf{x}_*)$ is contained within $\{E(\mathbf{x}) < c\}$.

Fix $\mathbf{x}(0) \in B_\delta(\mathbf{x}_*)$. We claim that the trajectory $\{\mathbf{x}(t) : t \geq 0\}$ can never enter the exterior of $E(\mathbf{x}) = c$. Suppose for a contradiction that there exists $t > 0$ such that $\mathbf{x}(t)$ is in the exterior of $E(\mathbf{x}) = c$. Then $E(\mathbf{x}(t)) > E(\mathbf{x}(0))$. As $E(\mathbf{x}(t))$ is smooth, the mean value theorem guarantees that there is a time $t_0 \in [0, t]$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t} E(\mathbf{x}(t))\bigg|_{t=t_0} > 0.$$

This contradicts that E is a weak Lyapunov function.

In particular, as $\{E(\mathbf{x}) \leq c\}$ is contained in $B_\epsilon(\mathbf{x}_*)$, then the trajectory remains in $B_\epsilon(\mathbf{x}_*)$.

(b) Fix $\mathbf{x}(0)$, and let $c = E(\mathbf{x}(0)) > 0$ so that $\mathbf{x}(0)$ lies in the level set $E(\mathbf{x}) = c$.

We claim that there are no equilibrium points other than $\mathbf{x}_*$ and no closed orbits. In the former case, we would have $\frac{\mathrm{d}}{\mathrm{d}t} E(\mathbf{x}(t)) = 0$ for all $t \geq 0$, which contradicts that E is a strong Lyapunov function. In the latter case, there would exist $t > 0$ such that $\mathbf{x}(t) = \mathbf{x}(0)$, and hence $E(\mathbf{x}(t)) = E(\mathbf{x}(0))$. As $E(\mathbf{x}(t))$ is smooth, the mean value theorem guarantees that there is a time $t_0 \in [0, t]$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t} E(\mathbf{x}(t))\bigg|_{t=t_0} = 0,$$

which contradicts that E is a strong Lyapunov function.

By the the Poincaré–Bendixson theorem (cf. [CL55, Ch. 16 Th. 2.1]), the only remaining possible behavior for the trajectory $\{\mathbf{x}(t) : t \geq 0\}$ is to approach $\mathbf{x}_*$. □

Next, we will examine the behavior of solutions in the limit where the friction term dominates. In this limit, the $\ddot{\mathbf{x}}$ term is negligible and we are often left with an equation of the form $\dot{\mathbf{x}} = -\nabla V(\mathbf{x})$. For the damped harmonic oscillator in Example 2.9 this is the limit $mk/b^2 \to 0$, which is rigorously justified in Exercise 2.4.

Definition 2.11. The ODE system (2.3) is a **gradient system** if there exists a smooth function V such that

$$\dot{\mathbf{x}} = -\nabla V(\mathbf{x}). \tag{2.5}$$

Although conservative systems $\ddot{\mathbf{x}} = -\nabla V(\mathbf{x})$ and gradient systems $\dot{\mathbf{x}} = -\nabla V(\mathbf{x})$ may look similar, they display nearly opposite behavior.

From multivariate calculus we know that the vector field $-\nabla V$ points in the direction of steepest descent for V and is orthogonal to the level sets of V. For our image of the ball rolling down the graph of the potential energy, the ball slows and never reaches the first minimum it encounters, as if the potential

energy graph were the bottom of a tank filled with water. Closed orbits are of course impossible again (cf. Exercise 2.5).

Example 2.12. In the over-damped limit for the harmonic oscillator we have

$$\dot{x} = -\tfrac{k}{b}x, \qquad V(x) = \tfrac{k}{2b}x^2.$$

This has the solution $x(t) = x_0 e^{-kt/b}$, which is the limiting (i.e. slow timescale) behavior for the over damped oscillator after the transient (i.e. fast timescale) behavior becomes negligible. In this limit, the trajectories in the phase portrait are confined to the line $p = m\dot{x} = -\frac{mk}{b}x$, which agrees with the fact that we can no longer take a second arbitrary initial condition $p(0)$ for the new one-dimensional system.

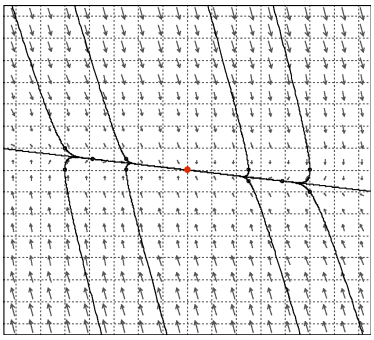


Figure 2.7: Phase portrait for the system of Example 2.12.

2.4. Time reversibility

In addition to a conserved quantity, conservative Newtonian systems also possess a symmetry in time. We will now give this property a name and study its mathematical consequences.

Definition 2.13. The ODE system (2.3) is (**time-**)**reversible** if there exists a smooth involution $\mathbf{R} : U \to U$ (i.e. $\mathbf{R}(\mathbf{R}(\mathbf{x})) = \mathbf{x}$ for all $\mathbf{x} \in U$) such that the change of variables $t \mapsto -t$, $\mathbf{x} \mapsto \mathbf{R}(\mathbf{x})$ leaves the system (2.3) invariant (i.e. if $\mathbf{x}(t)$ is a solution, then so is $\mathbf{R}(\mathbf{x}(-t))$).

Example 2.14. Consider a Newtonian system of the form

$$m\ddot{\mathbf{x}} = \mathbf{F}(\mathbf{x})$$

that is independent of time and velocity (or if $\mathbf{F}$ is even in velocity and time). Note that the force $\mathbf{F}$ does not have to be conservative. This system is invariant under the change of variables $t \mapsto -t$ since $\ddot{\mathbf{x}}$ picks up two factors of -1. Consequently, if $\mathbf{x}(t)$ is a solution then so is $\mathbf{x}(-t)$.

As a first-order system of ODEs in phase space, the involution is $\mathbf{R}(\mathbf{x}, \mathbf{p}) = (\mathbf{x}, -\mathbf{p})$. This tells us that trajectories in the phase portrait are symmetric across the position axes $\{(x_i, p_i) : p_i = 0\}$ with the time arrows on trajectories reversed.

Recall from Example 2.3 that when the linearized system (2.4) predicts that $\mathbf{x}_*$ is a center, we cannot conclude anything about the behavior of nearby solutions to the nonlinear system (2.3). In two dimensions however, reversibility is enough to recover this prediction:

Theorem 2.15 (Nonlinear centers for reversible systems)**.** *Suppose that the 2-dimensional ODE system* (2.3) *is reversible with* $\boldsymbol{R}$ *a reflection across a line, and that* $\mathbf{x}_*$ *is an isolated fixed point lying on the line of reflection. If the linearized system about* $\mathbf{x}_*$ *predicts a center, then all trajectories sufficiently close to* $\mathbf{x}_*$ *are closed.*

Proof. As $\mathbf{f}$ is smooth, Taylor's theorem guarantees that

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) = D\mathbf{f}(\mathbf{x}_*) \cdot (\mathbf{x} - \mathbf{x}_*) + \mathcal{O}\big(|\mathbf{x} - \mathbf{x}_*|^2\big).$$

By premise $\mathbf{x}_*$ is a linear center (cf. Example 2.2), and so solutions $\mathbf{y}(t)$ to the linearized equation

$$\dot{\mathbf{y}} = D\mathbf{f}(\mathbf{x}_*) \cdot (\mathbf{y} - \mathbf{x}_*)$$

are concentric ellipses centered at $\mathbf{x}_*$.

Fix $\mathbf{x}_0 \in B_\epsilon(\mathbf{x}_*)$ on the line of reflection. We claim there exists ϵ sufficiently small so that $\mathbf{x}(t)$ is never on the opposite side of $\mathbf{x}_*$ as $\mathbf{y}(t)$. Assuming this, the trajectory $\mathbf{x}(t)$ intersects the line of reflection on the other side of $\mathbf{x}_*$ at some time $t > 0$ because the trajectory $\mathbf{y}(t)$ encloses the origin. By reversibility, we can reflect this trajectory to obtain a twin trajectory with the same endpoints but with its arrow reversed. Taking $\epsilon > 0$ smaller if necessary, we can know that $\mathbf{x}_*$ is the only fixed point in $B_\epsilon(\mathbf{x}_*)$, and so the two trajectories together form a closed orbit.

It only remains to justify that such an $\epsilon > 0$ exists. Let $T > 0$ denote the period of solutions $\mathbf{y}(t)$ to the linearized system. Given an initial condition $\mathbf{x}_0$, define the difference

$$\mathbf{h}_t(\mathbf{x}_0) = \mathbf{x}(t) - \mathbf{y}(t)$$

at time $t \in [0, T]$ between the nonlinear and linear solutions starting at $\mathbf{x}_0$. The differential equations for $\mathbf{x}$ and $\mathbf{y}$ match to first order, and so we have

$$\mathbf{h}_t(0) = 0, \qquad D\mathbf{h}_t(0) = 0,$$

where D denotes the gradient in the spatial coordinates. As $\mathbf{f}$ is smooth, there exists a constant c so that

$$|D\mathbf{h}_t(\mathbf{x}_0)| \leq c \qquad \text{for all } \mathbf{x}_0 \in B_\epsilon(\mathbf{x}_*),\ t \in [0, T].$$

Moreover, $c \to 0$ as $\epsilon \downarrow 0$. Using the mean value theorem we estimate

$$|\mathbf{h}_t(\mathbf{x}_0)| = |\mathbf{h}_t(\mathbf{x}_0) - \mathbf{h}_t(0)| \leq c|\mathbf{x}_0| \qquad \text{for all } \mathbf{x}_0 \in B_\epsilon(\mathbf{x}_*),\ t \in [0, T].$$

The linear solutions $\mathbf{y}(t)$ are ellipses, and so there exists a constant $a > 0$ (depending on the semi-major and semi-minor axes) so that

$$|\mathbf{y}(t)| \geq a|\mathbf{y}(0)| = a|\mathbf{x}_0| \qquad \text{for all } t \in [0,T].$$

Combing the previous two inequalities, we conclude that there exists $\epsilon > 0$ sufficiently small so that

$$|\mathbf{x}(t) - \mathbf{y}(t)| = |\mathbf{h}_t(\mathbf{x}_0)| \leq \tfrac{1}{2}|\mathbf{y}(t)| \qquad \text{for all } \mathbf{x}_0 \in B_\epsilon(\mathbf{x}_*),\ t \in [0,T].$$

In other words, for $\mathbf{x}(0) = \mathbf{y}(0) \in B_\epsilon(\mathbf{x}_*)$ we have $|\mathbf{x}(t) - \mathbf{y}(t)| < |\mathbf{y}(t)|$ for all $t \in [0,T]$, and so $\mathbf{x}(t)$ is never on the opposite side of $\mathbf{x}_*$ as $\mathbf{y}(t)$. □

This argument can also be applied to specific examples to show the existence of individual closed, homoclinic, and heteroclinic orbits. The key input is establishing that the trajectory eventually reaches the hyperplane of symmetry, and then we can extend the trajectory using time-reversal symmetry.

Note that a general involution $\mathbf{R}$ can behave very differently in comparison to reflections, and so Theorem 2.15 does not clearly generalize to generic involutions. In particular, there may not be a hypersurface of fixed points; Exercise 2.8 provides a linear two-dimensional example where the symmetry only fixes one point.

2.5. Periodic motion

Consider a Newtonian system with one degree of freedom of the form

$$m\ddot{x} = F(x). \tag{2.6}$$

Any such system is conservative, because we can always find an antiderivative $-V(x)$ (unique up to an additive constant) so that $F = -V'(x)$. From Proposition 1.9 we know that the total energy

$$E = \tfrac{1}{2}m\dot{x}^2 + V(x) \tag{2.7}$$

is conserved by the motion. Note that (2.7) provides a first-order equation for $x(t)$ in place of the second-order equation (2.6). In this section, we will use this observation to solve for $x(t)$ and record some consequences.

Suppose that the potential $V(x)$ is shaped like a well, in the sense that $V(x) \to +\infty$ as $x \to \pm\infty$. The total energy (2.7) is conserved by Proposition 1.9, and hence $E(t) \equiv E$ is constant. The kinetic energy $\frac{1}{2}m\dot{x}^2$ is nonnegative, and so the solution $x(t)$ is confined to the region $\{x : V(x) \leq E\}$ in configuration space $\mathbb{R}_x$. This set is bounded since $V(x) \to +\infty$ as $x \to \pm\infty$, and so the motion is bounded.

By conservation of energy, the velocity $\dot{x}(t)$ vanishes for values of x with $V(x) = E$; these values are called the **turning points** of the motion. They are the two endpoints of the interval of $\{x : V(x) < E\}$ containing x_0, and they are the extremal points of the motion.

Most trajectories are periodic and oscillate between the two turning points. Indeed, if we have $V'(x) \neq 0$ at the two turning points, then the trajectory $x(t)$ reaches the turning point in finite time and doubles back. This is not true if $V'(x)$ vanishes at one of the turning points. One possibility is that the trajectory starts at an equilibrium point (x_0, p_0) in phase space, in which case we have $p_0 = 0$ and $V'(x_0) = 0$ so that $\dot{x} = 0$ and $\dot{p} = 0$ respectively. Alternatively, it could be that the turning point is an equilibrium, in which case the motion $x(t)$ approaches the turning point as $t \to \infty$ but never reaches it. Indeed, if $x(t)$ reaches the turning point then we have $\dot{x}(t) = 0$ by conservation of energy, but this violates the uniqueness of the equilibrium solution.

Suppose $x(t)$ is periodic with turning points $x_1(E) < x_2(E)$. Solving the energy equation (2.7) for $\dot{x}$ we obtain

$$\dot{x} = \sqrt{\tfrac{2}{m}[E - V(x)]}. \tag{2.8}$$

This is a separable differential equation with solution

$$t(E) = \sqrt{\frac{m}{2}} \int \frac{\mathrm{d}x}{\sqrt{E - V(x)}} + t_0.$$

The period τ is given by the integral from x_1 to x_2 to x_1, which is equivalent to two times the integral from x_1 to x_2:

$$\tau(E) = \sqrt{2m} \int_{x_1(E)}^{x_2(E)} \frac{\mathrm{d}x}{\sqrt{E - V(x)}}. \tag{2.9}$$

Altogether, we have proved the following:

Proposition 2.16. *Suppose the one-dimensional conservative Newtonian system* (2.6) *has a potential energy that obeys* $V(x) \to +\infty$ *as* $x \to \pm\infty$*. Then the motion* $x(t)$ *of the system is bounded. Moreover, when the motion is periodic the period is given by the integral* (2.9)*, where* E *is the initial energy and* $x_1(E) < x_2(E)$ *are the turning points of the motion.*

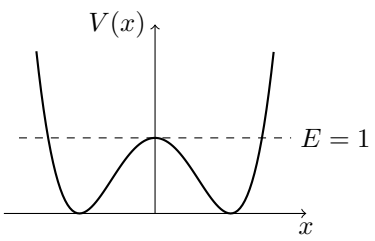
Example 2.17 (Double well)**.** Consider the system (2.6) with the double-well potential

$$V(x) = (x + 1)^2(x - 1)^2.$$

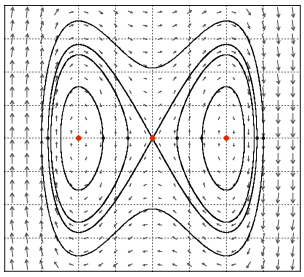
There are three equilibrium points in phase space: the two bottoms of the well, $(x_0, p_0) = (\pm 1, 0)$ with energy $E = 0$, and the unstable equilibrium $(x_0, p_0) = (0, 0)$ between the wells with energy $E = 1$. We know what the phase portrait looks like near these equilibria by the linear stability analysis of section 2.1, and we can use the level sets of the energy (2.7) to fill in the rest of the phase portrait.

For E in $(0, 1)$ or $(1, \infty)$ the motion is periodic. The turning points x_1, x_2 satisfy $V'(x_i) \neq 0$, and so nearby we have $V(x) \approx E + V'(x_i)(x - x_i)$. Consequently the integrand of (2.9) has a singularity $(x - x_i)^{-1/2}$ at both endpoints, and so the integral converges.

The level set $E = 1$ in phase space is comprised of three trajectories: the equilibrium $(0, 0)$ and two homoclinic orbits which are each traversed in an infinite amount of time. We have $V'(0) = 0$, and so near the turning point $x = 0$ we have $V(x) \approx E + \frac{1}{2}V''(0)x^2$. Consequently the integrand of (2.9) has a singularity x^{-1} at the endpoint $x = 0$, and so the integral diverges to $+\infty$.



(a) Potential energy.



(b) Phase portrait.

Figure 2.9: The system of Example 2.17.

The period of motion also has a geometric interpretation. Given a periodic trajectory at energy E, let $S(E)$ denote the area enclosed by the trajectory in the phase plane $\mathbb{R}_x \times \mathbb{R}_p$ with turning points $x_1 < x_2$. The system (2.6) is time-reversible, and so as in Example 2.14 the trajectory in phase space is symmetric about the x-axis. Therefore, expressing the top half of the curve $p = m\dot{x}$ as a function of position using (2.8), we may write the area as twice the area under the curve:

$$S(E) = 2\int_{x_1(E)}^{x_2(E)} \sqrt{2m[E - V(x)]}\,\mathrm{d}x.$$

Differentiate this using the Leibniz integral rule, we obtain

$$\begin{aligned}\frac{\mathrm{d}S}{\mathrm{d}E} &= 2\int_{x_1(E)}^{x_2(E)} \frac{\mathrm{d}}{\mathrm{d}E}\sqrt{2m[E - V(x)]}\,\mathrm{d}x \\ &\quad + 2\sqrt{2m[E - V(x_2)]}\,\frac{\mathrm{d}x_2}{\mathrm{d}E} - 2\sqrt{2m[E - V(x_1)]}\,\frac{\mathrm{d}x_1}{\mathrm{d}E}.\end{aligned}$$

As x_1, x_2 are turning points we know $V(x_1) = V(x_2) = E$, and so the second and third terms vanish. This yields

$$\frac{\mathrm{d}S}{\mathrm{d}E} = \sqrt{2m}\int_{x_1(E)}^{x_2(E)} \frac{\mathrm{d}x}{\sqrt{E - V(x)}}.$$

Comparing this expression to the period integral (2.9), we conclude:

Proposition 2.18. *For the system of Proposition 2.16, the period of a periodic trajectory is equal to the rate of change of the enclosed area with respect to energy:*

$$\tau(E) = \frac{\mathrm{d}S}{\mathrm{d}E}(E).$$

As a partial converse to Proposition 2.16, we will show that the period determines the shape of the potential:

Proposition 2.19. *For the system of Proposition 2.16, suppose that on an interval $(-r, r)$ the potential V has a minimum at $x = 0$, has no other critical points, and is even. Then all trajectories are periodic, and the potential V is uniquely determined (up to an additive constant) by the periods $\tau(E)$.*

Proof. By premise we have $V'(x) > 0$ for $x > 0$ and $V'(x) < 0$ for $x < 0$. This guarantees that all trajectories other than the equilibrium solution are periodic. As adding a constant does not change the equations of motion, we may assume that $V(0) = 0$. Each value $V > 0$ corresponds to exactly two values of x, which we will denote by $x_-(V) \in (-r, 0)$ and $x_+(V) \in (0, r)$. Changing variables in the period integral (2.9), we obtain

$$\begin{aligned}\tau(E) &= \sqrt{2m}\int_{x_1(E)}^{0} \frac{\mathrm{d}x}{\sqrt{E - V(x)}} + \sqrt{2m}\int_{0}^{x_2(E)} \frac{\mathrm{d}x}{\sqrt{E - V(x)}} \\ &= \sqrt{2m}\int_0^E \left(\frac{\mathrm{d}x_+}{\mathrm{d}V} - \frac{\mathrm{d}x_-}{\mathrm{d}V}\right) \frac{\mathrm{d}V}{\sqrt{E - V}}.\end{aligned}$$

We divide both sides by $\sqrt{W - E}$ and integrate with respect to E from 0 to W:

$$\begin{aligned}&\int_0^W \frac{\tau(E)\,\mathrm{d}E}{\sqrt{W - E}} = \sqrt{2m}\int_0^W \int_0^E \left(\frac{\mathrm{d}x_+}{\mathrm{d}V} - \frac{\mathrm{d}x_-}{\mathrm{d}V}\right) \frac{\mathrm{d}V\,\mathrm{d}E}{\sqrt{(W - E)(E - V)}} \\ &= \sqrt{2m}\int_0^W \left(\frac{\mathrm{d}x_+}{\mathrm{d}V} - \frac{\mathrm{d}x_-}{\mathrm{d}V}\right) \left[\int_V^W \frac{dE}{\sqrt{(W - E)(E - V)}}\right] \mathrm{d}V \\ &= \pi\sqrt{2m}\int_0^W \left(\frac{\mathrm{d}x_+}{\mathrm{d}V} - \frac{\mathrm{d}x_-}{\mathrm{d}V}\right) \mathrm{d}V = \pi\sqrt{2m}\,[x_+(W) - x_-(W)]\,.\end{aligned}$$

In the last equality we noted $x_\pm(0) = 0$. Taking $W = V$ we obtain

$$x_+(V) - x_-(V) = \frac{1}{\pi\sqrt{2m}}\int_0^V \frac{\tau(E)}{\sqrt{V - E}}\,\mathrm{d}E.$$

In this way, the period determines the potential energy. □

2.6. Exercises

2.1 (Pendulum)**.** Consider a mass m attached to the end of a rigid massless rod of length ℓ with the other end suspended at a fixed point. We allow the rod to rotate in a vertical plane, subject to a constant downward gravitational acceleration g.

(a) Let x denote the angle from the vertical directly below the pivot, and show that

$$\ddot{x} = -\tfrac{g}{\ell}\sin x.$$

(We have not allowed for configuration spaces other than Euclidean space yet, so at the moment we are simply viewing $x \in \mathbb{R}$.)

(b) Sketch the potential energy and the phase portrait, and convince yourself that the trajectories correspond to a small ball rolling down the graph of the potential (cf. section 1.4). Note that near the origin in the phase plane the diagram looks like that of the harmonic oscillator (cf. Example 2.2), which is a consequence of the small-angle approximation $\sin x \approx x$. Identify all equilibria and heteroclinic orbits. How many trajectories make up the eye-shaped energy level set from $-\pi \leq x \leq \pi$ that separates different modes of behavior, and to what motion do they correspond?

(c) Now add a damping term:

$$\ddot{x} = -b\dot{x} - \tfrac{g}{\ell} \sin x$$

where $b > 0$. Show that $\frac{\mathrm{d}}{\mathrm{d}t} E \leq 0$ along all trajectories, and sketch the new phase portrait.

2.2 (Non-mechanical conservative system)**.** Consider the Lotka–Volterra model

$$\dot{x} = x(1 - y), \qquad \dot{y} = \mu y(x - 1)$$

for a predator-prey system, where $\mu > 0$ is a constant parameter.

(a) Use the chain rule to find a differential equation for $\frac{\mathrm{d}y}{\mathrm{d}x}$.

(b) Integrate this separable differential equation to find a conserved quantity $E(x, y)$ for the system.

(c) Show that all trajectories are periodic for initial conditions $x(0), y(0) > 0$.

2.3 (Conserved quantity minimum that is not a center)**.** Consider the system

$$\dot{x} = xy, \qquad \dot{y} = -x^2.$$

Show that $E(x, y) = x^2 + y^2$ is a conserved quantity and plot the phase portrait for this system. Although the origin is a minimum for E, it is not an isolated fixed point nor a center.

2.4 (Over-damped limit for the harmonic oscillator)**.** We will now justify the over-damped limit approximation in Example 2.12. The objective is to find a regime for the damped harmonic oscillator

$$m\ddot{x} = -b\dot{x} - kx, \qquad b, k > 0$$

in which the $\ddot{x}$ term is negligible.

(a) By equating the units of each term in the differential equation, determine the units of b and k. (Assume that x is measured in units of, say, length.)

(b) Define a new dimensionless variable τ via $t = T\tau$, where T is a constant with units time to be chosen. Find the new differential equation in terms of τ. Pick T to make the coefficient of the $\dot{x}$ term equal to one, and check that T has units time.

(c) The coefficient of the $\ddot{x}$ term should be mk/b^2, and so the limit in which this term is negligible is $\epsilon = mk/b^2 \to 0$. Find the general solution $x(t) = c_1 e^{k_1 t} + c_2 e^{k_2 t}$ for the linear equation $\epsilon\ddot{x} + \dot{x} + x = 0$.

(d) Recall that $1/|k|$ is called the characteristic time of e^{kt}, because after a time $1/|k|$ the function has decreased (since $k < 0$) by a factor of $1/e$. Find the leading term in the Taylor expansion of $1/k_1$ and $1/k_2$ about $\epsilon = 0$; these are called the fast and slow timescales for the solution.

2.5. Show that nonconstant periodic solutions are impossible in a gradient system by considering the change in $V(\mathbf{x})$ around such an orbit. Conclude that any one-dimensional first order ODE has no periodic solutions.

2.6 (Low-regularity existence for gradient systems [San17])**.** The special form of gradient systems allows us to establish existence and uniqueness with fewer regularity assumptions. This is particularly useful for gradient PDE systems, where $\mathbb{R}^n$ is replaced by an infinite-dimensional function space.

Suppose $F : \mathbb{R}^n \to \mathbb{R}$ is a convex (and not necessarily smooth) function. This guarantees that the sub-differential

$$\partial F(\mathbf{x}) = \{\mathbf{v} \in \mathbb{R}^n : F(\mathbf{y}) \geq F(\mathbf{x}) + \mathbf{v} \cdot (\mathbf{y} - \mathbf{x}) \text{ for all } \mathbf{y} \in \mathbb{R}^n\}$$

is nonempty for each $\mathbf{x} \in \mathbb{R}^n$. Note that F is differentiable at $\mathbf{x}$ if and only if $\partial F(\mathbf{x}) = \{\nabla F(\mathbf{x})\}$. For $\mathbf{x} : [0, \infty) \to \mathbb{R}^n$ absolutely continuous, consider the gradient system

$$\dot{\mathbf{x}}(t) \in -\partial F(\mathbf{x}(t)) \quad \text{for almost every } t > 0, \qquad \mathbf{x}(0) = \mathbf{x}_0.$$

(a) Prove uniqueness of solutions by differentiating the squared difference of two solutions.

(b) Fix $\tau > 0$, and recursively define the sequence

$$\mathbf{x}_0^\tau = \mathbf{x}_0, \qquad \mathbf{x}_{k+1}^\tau \text{ a minimizer of } \mathbf{x} \mapsto F(\mathbf{x}) + \tfrac{1}{2\tau}|\mathbf{x} - \mathbf{x}_k^\tau|^2.$$

Show that

$$\tfrac{1}{\tau}\left[\mathbf{x}_{k+1}^\tau - \mathbf{x}_k^\tau\right] \in -\partial F(\mathbf{x}_{k+1}^\tau).$$

For F differentiable, this is simply the implicit Euler scheme for $\dot{\mathbf{x}} = -\nabla F(\mathbf{x})$.

(c) In order to extract a convergent sequence as $\tau \downarrow 0$, we need a compactness estimate. Use the definition of the sequence $\mathbf{x}_k^\tau$ show that

$$\sum_{k=0}^{K} \tfrac{1}{2\tau}|\mathbf{x}_{k+1}^\tau - \mathbf{x}_k^\tau|^2 \leq F(\mathbf{x}_0) - F(\mathbf{x}_{K+1}^\tau).$$

(d) Define the piecewise constant and linear interpolations

$$\mathbf{x}^\tau(t) = \mathbf{x}_{k+1}^\tau, \quad \widetilde{\mathbf{x}}^\tau(t) = \mathbf{x}_k^\tau + \tfrac{\mathbf{x}_{k+1}^\tau - \mathbf{x}_k^\tau}{\tau}(t - k\tau) \quad \text{for } t \in (k\tau, (k+1)\tau].$$

Use the previous part to show there exists a constant C such that

$$\int_0^T \tfrac{1}{2}|(\widetilde{\mathbf{x}}^\tau)'(t)|^2 \,\mathrm{d}t \le C.$$

Conclude that

$$|\widetilde{\mathbf{x}}^\tau(t) - \widetilde{\mathbf{x}}^\tau(s)| \le C|t-s|^{1/2}, \qquad |\widetilde{\mathbf{x}}^\tau(t) - \mathbf{x}^\tau(t)| \le C\tau^{1/2}.$$

(e) Assume that F is bounded below. For any $T > 0$, use the Arzelà–Ascoli theorem to show that $\widetilde{\mathbf{x}}^\tau : [0,T] \to \mathbb{R}^n$ admits a uniformly convergent subsequence as $\tau \downarrow 0$, and that $\mathbf{x}^\tau$ converges uniformly to the same limit. After passing to a further subsequence if necessary, show that $(\widetilde{\mathbf{x}}^\tau)'$ converges weakly in $L^2([0,T])$. Conclude that the limit $\mathbf{x}(t)$ solves the gradient system for F.

2.7 (Gradient flows in PDE)**.** For $u : \mathbb{R}^n \to \mathbb{R}$ define the Dirichlet energy

$$E(u) = \begin{cases} \frac{1}{2}\int |\nabla u(x)|^2 \,\mathrm{d}x & \text{if } \nabla u \in L^2, \\ +\infty & \text{else.} \end{cases}$$

In analogy with directional derivatives for functions on $\mathbb{R}^n$, the gradient $\nabla E(u)$ of the functional E at u is defined by

$$\frac{\mathrm{d}}{\mathrm{d}s} E(u+sv)\bigg|_{s=0} = \langle \nabla E(u), v\rangle \quad \text{for all } v,$$

when it exists. Different choices of inner products on the RHS yields different notions of gradients.

(a) For the inner product

$$\langle u, v\rangle_{L^2} = \int u(x)v(x)\,\mathrm{d}x$$

on $L^2(\mathbb{R}^n;\mathbb{R})$, show that formally the gradient flow for the energy E is the heat equation

$$\frac{\partial u}{\partial t} = -\Delta u.$$

(b) For the inner product

$$\langle u, v\rangle_{\dot{H}^1} = \int \nabla u(x)\cdot\nabla v(x)\,\mathrm{d}x$$

on $\dot{H}^1(\mathbb{R}^n;\mathbb{R}) = \{u : \mathbb{R}^n \to \mathbb{R} : \int |\nabla u|^2\,\mathrm{d}x < \infty\}$, show that formally the gradient flow for the energy E is the equation

$$\frac{\partial u}{\partial t} = -u.$$

Note that the higher regularity norm yields less regular solutions: it is well-known that solutions to the heat equation are automatically smooth, while solutions $u(t,x) = e^{-t}u_0(x)$ to this equation are only as smooth as the initial data.

2.8 (A non-mechanical reversible system)**.** Show that the system

$$\dot{x} = -2\cos x - \cos y, \qquad \dot{y} = -2\cos y - \cos x$$

is reversible with respect to rotation by π. Note that the presence of stable and unstable nodes guarantees that this system is not conservative.

2.9 (Pendulum period)**.** Show that for the pendulum

$$\ddot{x} = -\tfrac{g}{\ell}\sin x,$$

the motion with turning points $\pm\theta_0$ has period

$$\tau = 4\sqrt{\tfrac{\ell}{g}}K\big(\sin\tfrac{\theta_0}{2}\big),$$

where

$$K(k) = \int_0^{\pi/2} \frac{\mathrm{d}\xi}{\sqrt{1-k^2\sin^2\xi}}$$

is the complete elliptic integral of the first kind. By Taylor expanding about $\theta_0 = 0$, find the expansion:

$$\tau \approx 2\pi\sqrt{\tfrac{\ell}{g}}\left(1 + \tfrac{1}{16}\theta_0^2 + \ldots\right).$$

Note that the zeroth order term is the constant-period approximation obtained by taking $\sin x \approx x$ and thus replacing the pendulum by a harmonic oscillator.

2.10 (Existence of solitons)**.** In 1844, Scott Russell famously observed a solitary traveling wave (now commonly referred to as a *soliton*) in a canal, contradicting the popular belief that all water waves must either crest and break or disperse. In order to explain this phenomenon, the Korteweg–de Vries equation

$$\frac{\partial u}{\partial t} = -\frac{\partial^3 u}{\partial x^3} - 6u\frac{\partial u}{\partial x}$$

was introduced in [KdV95] as a model for the surface $u : \mathbb{R}_t \times \mathbb{R}_x \to \mathbb{R}$ of a shallow channel of water.

(a) We seek traveling wave solutions to this PDE. Insert the ansatz $u(t,x) = h(x-ct)$ where $c > 0$ is a constant and obtain an ODE for $h(x)$.

(b) Integrate the equation for h once to obtain a second-order ODE, and write it in the form $\frac{\mathrm{d}^2h}{\mathrm{d}x^2} = -V'(h)$ of a conservative mechanical system for some potential function $V(h)$.

(c) Use the conserved quantity $\frac{1}{2}(h')^2 + V(h)$ to sketch the phase portrait in the (h, h')-plane. Highlight a unique homoclinic orbit connecting the fixed point at the origin to itself; the corresponding solution $h(x)$ obeys $h(x) \to 0$ as $x \to \pm\infty$, and thus describes the profile of a localized wave.

(d) Use the conservation of $\frac{1}{2}(h')^2 + V(h)$ to obtain a first-order ODE for h. This equation is separable, and thus can be integrated. Conclude that solitary traveling wave solutions are given by the formula

$$u(t, x) = 2\beta^2 \operatorname{sech}^2 \left[\beta(x - x_0 - 4\beta^2 t)\right]$$

for arbitrary constants $x_0 \in \mathbb{R}$ and $\beta > 0$. How is the speed of these waves related to their amplitude?

CHAPTER 3

CENTRAL FIELDS

We will examine some examples of systems with more than one degree of freedom. This selection focuses on the most important examples in order to provide a baseline intuition; a thorough study of classical mechanics should include many more examples, e.g. rigid bodies and the mechanical top. The material is based on [Arn89, Ch. 2], [LL76, Ch. 3], and [Gol51, Ch. 3].

3.1. Central fields

In this section we will solve for the motion of a single particle in $\mathbb{R}^3$ subject to a central force $\mathbf{F}$. A vector field $\mathbf{F}$ is called **central** (about the origin) if all of the vectors are radial and the magnitude is only a function of the radial coordinate $r = |\mathbf{x}|$; in other words, $\mathbf{F} \equiv F(r)\hat{\mathbf{r}}$. (This definition of course extends to $\mathbb{R}^d$, but soon we will need to specialize to $\mathbb{R}^3$ in order to discuss angular momentum.)

A central field must be conservative, and the corresponding potential energy $V \equiv V(r)$ depends only on the distance to the origin. This is because $F(r)$ is a function of one variable and thus we can always find an antiderivative $-V(r)$. Alternatively, if we write $\mathbf{F} = F(r)\hat{\mathbf{r}}$, then the work

$$\int_{\mathbf{x}_1}^{\mathbf{x}_2} \mathbf{F} \cdot \mathrm{d}\mathbf{s} = \int_{|\mathbf{x}_1|}^{|\mathbf{x}_2|} F(r)\,\mathrm{d}r$$

is path independent and so from Proposition 1.7 we know there exists a radial potential energy $V(r)$ so that $\mathbf{F} = -\nabla V$.

The torque of the particle is

$$\mathbf{N} = \mathbf{x} \times \mathbf{F} = F(r)r(\hat{\mathbf{r}} \times \hat{\mathbf{r}}) = 0,$$

and so by Proposition 1.16 we know the particle's angular momentum $\mathbf{L} = \mathbf{x} \times \mathbf{p}$ is conserved. As $\mathbf{x}$ is always perpendicular to $\mathbf{L}$, we see that the particle's motion is confined to the plane orthogonal to $\mathbf{L}$ provided that $\mathbf{L} \neq 0$ initially. If $\mathbf{L} = 0$, then $\mathbf{x}$ is parallel to the velocity $\dot{\mathbf{x}}$, and thus the particle's motion must be collinear. In both cases, the motion is coplanar.

As a consequence of the conservation of angular momentum, we have:

Proposition 3.1 (Kepler's second law)**.** *The rate of change in the total area swept by the radius vector as a function of time is constant.*

Proof. Let (r, ϕ) denote polar coordinates within the plane of motion. The velocity in these coordinates is

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} r\cos\phi \\ r\sin\phi \end{pmatrix} = \dot{r}\begin{pmatrix} \cos\phi \\ \sin\phi \end{pmatrix} + r\dot{\phi}\begin{pmatrix} -\sin\phi \\ \cos\phi \end{pmatrix} = \dot{r}\hat{\mathbf{r}} + r\dot{\phi}\hat{\boldsymbol{\phi}}.$$

The magnitude L of the angular momentum $\mathbf{L}$ is then

$$L = |\mathbf{x} \times \mathbf{p}| = |(r\hat{\mathbf{r}}) \times (m\dot{\mathbf{x}})| = mr^2\dot{\phi}. \tag{3.1}$$

Note that the conservation of L requires that $\dot{\phi}$ cannot change sign.

On the other hand, the area ΔS of the angular wedge swept by the radius vector $\mathbf{x}$ over an angle $\Delta\phi$ is given by

$$\Delta S = \tfrac{1}{2}\mathbf{x} \cdot \mathbf{x}\Delta\phi + \mathcal{O}(\Delta\phi^2) = \tfrac{1}{2}r^2\dot{\phi}\Delta t + \mathcal{O}(\Delta t^2)$$

to first order. Together, we see that the total area $S(t)$ swept by the radius vector obeys

$$\dot{S} = \tfrac{1}{2}r^2\dot{\phi} = \tfrac{1}{2m}L \tag{3.2}$$

and thus is constant. □

Using (3.1), we can rewrite the total energy as

$$E = K + V = \tfrac{m}{2}(\dot{r}^2 + r^2\dot{\phi}^2) + V(r) = \tfrac{m}{2}\dot{r}^2 + \tfrac{L^2}{2m}r^{-2} + V(r). \tag{3.3}$$

This is the total energy for a one-dimensional Newtonian system in the coordinate r with the **effective potential** energy

$$V_{\text{eff}}(r) = V(r) + \tfrac{L^2}{2m}r^{-2}.$$

The last term on the RHS is called the **centrifugal energy**. When the effective potential is equal to the total energy we have $\dot{r} = 0$, which is a turning point for the one-dimensional system. Unlike in section 2.5 though, the actual particle is not at rest at such a point because the angle is changing (unless the angular momentum is zero).

Example 3.2. Kepler's problem seeks the equations of motion for a particle moving around a fixed gravitational mass, which is governed by the potential

$$V(r) = -kr^{-1}$$

for $k > 0$ a constant. This yields the effective potential

$$V_{\text{eff}}(r) = -kr^{-1} + \tfrac{L^2}{2m}r^{-2}.$$

The potential $V(r)$ tends to $-\infty$ as $r \downarrow 0$, but the added centrifugal energy makes the effective potential $V_{\text{eff}}(r)$ tend to $+\infty$.

If the initial energy E_0 is nonnegative, then the trajectory is unbounded. The particle comes in from infinity, swings around the central mass reaching a minimum radius where $V_{\text{eff}} = E_0$, and returns towards infinity.

If the initial energy E_0 is negative, then the trajectory is bounded. The particle moves within an annulus, oscillating between the inner and outer radii where $V_{\text{eff}} = E_0$. As of yet we do not know if the trajectory is periodic, never realigns, or even is dense in the annulus.

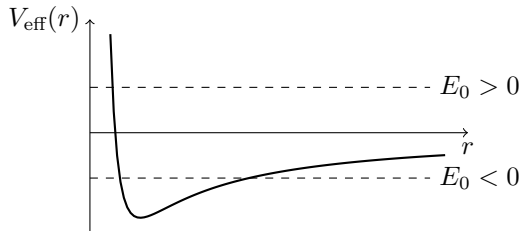


Figure 3.1: Effective potential for the system of Example 3.2.

Rearranging the total energy (3.3), we obtain

$$\dot{r} = \sqrt{\tfrac{2}{m}[E - V_{\text{eff}}(r)]}. \tag{3.4}$$

This is a separable differential equation, with solution

$$t = \int \frac{\mathrm{d}r}{\sqrt{\tfrac{2}{m}[E - V_{\text{eff}}(r)]}} + t_0. \tag{3.5}$$

We can also use the expression (3.4) for $\dot{r}$ to solve the separable equation (3.1) for ϕ:

$$\phi = \int \frac{L\,\mathrm{d}r}{r^2\sqrt{2m[E - V_{\text{eff}}(r)]}} + \phi_0. \tag{3.6}$$

This is a formula for ϕ as a function of r, at least formally.

The original system of differential equations was six-dimensional: 3 dimensions for the position $\mathbf{x} \in \mathbb{R}^3$ and 3 dimensions for the momentum $\mathbf{p} \in \mathbb{R}^3$. We then used 4 conserved quantities to reduce the system to 2 first-order equations, which could then be integrated. Indeed, the conservation of the angle of $\mathbf{L}$ eliminated 2 degrees of freedom by restricting the motion to be coplanar, and the conservation of the magnitude of $\mathbf{L}$ eliminated another degree of freedom by providing the first-order equation (3.1) for ϕ. The fourth conserved quantity was the total energy E, which we used to obtain the first-order equation (3.4) for r.

As in section 2.5, the motion is confined to the region $V_{\text{eff}} \leq E$. Nevertheless, in general the particle may still be able to approach $r = \infty$. Indeed, if the potential energy at infinity $V_\infty = \lim_{r\to\infty} V(r) = \lim_{r\to\infty} V_{\text{eff}}(r)$ exists and is

finite, then there are unbounded trajectories for energies $E \geq V_\infty$ and we can define the velocity at infinity $v_\infty \geq 0$ via $E = \frac{1}{2}mv_\infty^2 + V_\infty$. On the other hand, the particle may also be able to approach $r = 0$. In order for this to happen, the potential $V(r)$ must not outgrow the centrifugal energy:

$$\limsup_{r \downarrow 0} \left[V(r) + \tfrac{L^2}{2m} r^2 \right] < +\infty.$$

In the remaining case, the effective potential has two turning points $r_{\min}$ and $r_{\max}$, which confines the motion within the annulus bounded by these two radii. Points where $r = r_{\min}$ are called **pericenters** and points where $r = r_{\max}$ are called **apocenters**. The time symmetry for the one-dimensional system in r implies that the trajectory will be symmetric about any ray from the origin through a pericenter or apocenter. According to the solution (3.6), the angle between successive pericenters (or apocenters) is then

$$\Phi = 2 \int_{r_{\min}}^{r_{\max}} \frac{L \, \mathrm{d}r}{r^2 \sqrt{2m[E - V_{\text{eff}}(r)]}}. \tag{3.7}$$

In general, Φ is not a rational multiple of 2π, and consequently the trajectory is not closed (and, it turns out, is necessarily dense in the annulus).

3.2. Periodic orbits

We have seen two special examples of central fields thus far: the harmonic oscillator potential

$$V(r) = kr^2, \qquad k > 0, \tag{3.8}$$

and the gravitational potential

$$V(r) = -kr^{-1}, \qquad k > 0. \tag{3.9}$$

The objective of this section is to show that these are the only two central fields for which all bounded orbits are periodic:

Theorem 3.3 ([Arn89, §8D])**.** *Suppose a particle moves in a smooth central field on $\mathbb{R}^3 \setminus \{0\}$ and there exists a bounded trajectory. If all bounded trajectories are periodic, then the potential is either the harmonic oscillator potential* (3.8) *or the gravitational potential* (3.9)*.*

For $V(r) = -kr^p$ with $p \in (-2, 0)$, the effective potential still has the same qualitative shape as in the case $p = -1$ from Example 3.2: $V_{\text{eff}}(r) \to +\infty$ as $r \downarrow 0$ and $V_{\text{eff}}(r) \to 0$ as $r \to \infty$, with a negative minimum in between. If $p \neq -1$, Theorem 3.3 implies that for $E_0 < 0$ there must be trajectories that are not periodic. In fact, it can be shown that such trajectories are dense in the annulus $\{r : V_{\text{eff}}(r) \leq E_0\}$.

To begin the proof of Theorem 3.3, suppose $V(r)$ is a central field in which all bounded orbits are closed. The existence of a closed orbit guarantees that

$V_{\text{eff}}(r)$ has a (strict) local minimum at some value $r > 0$. Indeed, if $V'_{\text{eff}}(r) < 0$ for all $r > 0$, then we eventually have $V_{\text{eff}}(r) \leq E_0 - a$ for some $a > 0$ and all t large, and hence $\dot{r} \leq b > 0$ for all t large by conservation energy. Similarly, if $V'_{\text{eff}}(r) > 0$ for all $r > 0$, then we eventually have $V_{\text{eff}}(r) \leq E_0 - a$ for some $a > 0$ and all t large, and hence $\dot{r} \leq -b < 0$ for all t large by conservation energy. In either case, we eventually have that $\dot{r}$ is nonvanishing, and so no closed orbits could exist.

Let r_0 denote a local minimum of V_{eff}. If the initial radius is sufficiently close to r_0 then the energy E_0 will be close to $V_{\text{eff}}(r_0)$ and the motion will be confined to a bounded component of $\{r : V(r) \leq E_0\}$. From (3.7), the angle between successive pericenters or apocenters is

$$\Phi = 2 \int_{r_{\min}}^{r_{\max}} \frac{L}{r^2 \sqrt{2m[E - V(r) - L^2/2mr^2]}} \, \mathrm{d}r,$$

where $r_{\min}$ and $r_{\max}$ are the radial turning points. Substituting $x = \frac{L}{mr}$, we obtain

$$\Phi = \sqrt{2m} \int_{x_{\min}}^{x_{\max}} \frac{1}{\sqrt{E - V(L/mx) - mx^2/2}} \, \mathrm{d}x. \tag{3.10}$$

This is the period integral (2.9) for the one-dimensional system with potential

$$W(x) = V\left(\tfrac{L}{mx}\right) + \tfrac{m}{2}x^2.$$

Next, we compute the limiting period for small oscillations near minima for the one-dimensional system with potential W:

Lemma 3.4. *Consider a conservative one-dimensional Newtonian system with smooth potential $W(x)$. If W has a local minimum x_0 with value E_0, then*

$$\lim_{E \downarrow E_0} \tau(E) = 2\pi \sqrt{\tfrac{m}{W''(x_0)}}. \tag{3.11}$$

Proof. After substituting $W - E_0$ for W we may assume that $E_0 = 0$. As x_0 is a local minimum with value 0, the Taylor expansion of W at x_0 is

$$W(x) = \tfrac{1}{2}W''(x_0)(x - x_0)^2 + \mathcal{O}\big((x - x_0)^3\big).$$

This yields the equations of motion

$$m\ddot{x} = -W''(x_0)(x - x_0) + \mathcal{O}\big((x - x_0)^2\big).$$

Without the error term, this is a harmonic oscillator about x_0 with spring constant $k = W''(x_0)$, and in Example 2.2 we found that the solution can be expressed in terms of trigonometric functions with period

$$2\pi \sqrt{\tfrac{m}{k}} = 2\pi \sqrt{\tfrac{m}{W''(x_0)}}.$$

This gives us the formula (3.11) for the leading term of $\tau(E)$ as $E \downarrow E_0$. The convergence of $\tau(E)$ as $E \downarrow E_0$ can be justified by passing the limit inside the integral expression (2.9). □

Let r_0 denote a local minimum of V_{eff}. Then W has a minimum at

$$x_0 = \tfrac{L}{mr_0}.$$

Consequently we have $W'(x_0) = 0$, which yields

$$m^2 x_0^3 = LV'(r_0).$$

Inserting this into the expression for $W''(x_0)$, we obtain

$$W''(x_0) = m\frac{r_0 V''(r_0) + 3V'(r_0)}{V'(r_0)}.$$

Therefore, taking the limit $E \downarrow V(r_0)$ in the angle integral (3.10) and applying (3.11), we conclude that the angle Φ tends to

$$\Phi_{\text{cir}} = 2\pi\sqrt{\frac{m}{W''(x_0)}} = 2\pi\sqrt{\frac{V'(r_0)}{r_0 V''(r_0) + 3V'(r_0)}} \tag{3.12}$$

as the initial radius tends to r_0.

All of the orbits near r_0 are bounded, and so by premise they must be closed. As Φ is the angle between successive pericenters or apocenters, some integer multiple of Φ must be equal to $2\pi n$ for some integer $n \geq 1$. Therefore Φ is a rational multiple of 2π, and since the integral is a continuous function of the initial condition in a neighborhood of r_0 then we must have $\Phi = \Phi_{\text{cir}}$ on this neighborhood of r_0. Setting (3.12) equal to a constant, we obtain the linear differential equation

$$cr_0 V''(r_0) + (3c - 1)V'(r_0) = 0$$

for $c \in \mathbb{R}$ a constant. The solutions are

$$V(r) = ar^\alpha \text{ for } \alpha \in [-2, 0) \cup (0, \infty), \quad \text{and} \quad V(r) = b \log r,$$

and in both cases Φ is constant. Plugging this back into Φ_{cir}, we obtain

$$\Phi \equiv \Phi_{\text{cir}} = \tfrac{2\pi}{\sqrt{\alpha+2}} \quad \text{for } \alpha \geq -2. \tag{3.13}$$

(The case $\alpha = 0$ corresponds to $V(r) = b \log r$.) We will now split into cases.

First consider the case $V(r) = b \log r$. Taking $\alpha = 0$ in (3.13) we have $\Phi_{\text{cir}} = \sqrt{2}\pi$, and so Φ is not a rational multiple of 2π.

Next, consider the case $V(r) = ar^\alpha$ with $\alpha > 0$. The constant a must be positive so that there exists a bounded orbit, and hence $V(r) \to \infty$ as $r \to \infty$. Substituting $x = x_{\max} y$ in the Φ integral (3.10), we have

$$\Phi = \sqrt{2m}\int_{y_{\min}}^{1} \frac{\mathrm{d}y}{\sqrt{U(1) - U(y)}}, \qquad U(y) = \frac{my^2}{2} + \frac{1}{x_{\max}^2} V\left(\frac{L}{mx_{\max} y}\right).$$

As $E \to \infty$ we have $x_{\max} \to \infty$ and the second term in U tends to zero. Moreover, in this limit we also have $y_{\min} \to 0$ and so we obtain

$$\lim_{E\to\infty} \Phi = \pi.$$

On the other hand, $\Phi \equiv \Phi_{\text{cir}}$ is a constant, and so comparing to (3.13) we conclude that $\alpha = 2$.

Now consider the case $V(r) = ar^\alpha$ with $-2 \le \alpha < 0$. Taking the limit $E \downarrow 0$ in the integral (3.10), we obtain

$$\lim_{E\downarrow 0} \Phi = 2\int_0^1 \frac{\mathrm{d}x}{\sqrt{x^{-\alpha} - x^2}} = \frac{2\pi}{2+\alpha}.$$

Comparing this to (3.13), we conclude $\alpha = -1$.

Altogether, the only two possible potentials are the harmonic oscillator (3.8) and the gravitational potential (3.9). This concludes the proof of Theorem 3.3.

3.3. Kepler's problem

Kepler's problem seeks the motion for the central field with potential

$$V(r) = -kr^{-1}, \qquad k > 0.$$

The original motivation was to model a celestial body in motion around a fixed gravitational object, but this also describes the motion of an electrically charged particle attracted to a fixed charge.

From section 3.1 we know the motion is coplanar, and the radius r evolves subject to the one-dimensional effective potential

$$V_{\text{eff}}(r) = -kr^{-1} + \tfrac{L^2}{2m} r^{-2}.$$

Note that $\lim_{r\downarrow 0} V_{\text{eff}}(r) = +\infty$ and $\lim_{r\to\infty} V_{\text{eff}}(r) = 0$. If $L \neq 0$ then the first derivative

$$V'_{\text{eff}}(r) = \tfrac{k}{r^2} - \tfrac{L^2}{mr^3}$$

has exactly one root for $r \in (0,\infty)$ at $r = L^2/mk$, and so V_{eff} has a strict global minimum with value

$$V_{\text{eff}}\left(\tfrac{L^2}{mk}\right) = -\tfrac{mk^2}{2L^2}.$$

Consequently, for $E \ge 0$ we have unbound motion, and for $E < 0$ (with $L \neq 0$) we have bounded motion with $E \ge -\frac{mk^2}{2L^2}$.

For this potential we can evaluate the formal solution (3.6) for the angular coordinate:

$$\phi(r) = \cos^{-1}\left(\frac{\frac{L}{r} - \frac{mk}{L}}{\sqrt{2mE + \frac{m^2k^2}{L^2}}}\right).$$

Given an initial condition, we picked the origin for ϕ so that integration constant above is zero. Solving for r as a function of ϕ, we obtain

$$r = \frac{L^2/mk}{1 + \sqrt{1 + 2EL^2/mk^2}\,\cos\phi}.$$

Define the quantities

$$\ell = \tfrac{L^2}{mk}, \qquad \epsilon = \sqrt{1 + \tfrac{2EL^2}{mk^2}},$$

so that we may write

$$r(\phi) = \frac{\ell}{1 + \epsilon\cos\phi}.$$

This is the parametric equation for a conic section having one focus at the origin, with eccentricity $\epsilon \in [0, \infty)$ and latus rectum 2ℓ. By planar geometry, the semi-major and semi-minor axes are given by

$$a = \frac{\ell}{1-\epsilon^2} = \frac{k}{2|E|}\ , \qquad b = \frac{\ell}{\sqrt{1-\epsilon^2}} = \frac{L}{\sqrt{2m|E|}}, \tag{3.14}$$

respectively.

The eccentricities $\epsilon = 1$ and $\epsilon > 1$ correspond to parabolas and hyperbolas respectively, which agrees with the fact that $E \geq 0$ yields unbound orbits. Likewise $\epsilon = 0$ and $0 < \epsilon < 1$ correspond to circles and ellipses respectively, which agrees with the fact that $E \in [-\frac{mk^2}{2L^2}, 0)$ yields bounded orbits.

For the planets in our solar system, the eccentricities are very small and the trajectories are nearly circular. Consequently, before solving Kepler's problem, scientists (such as Copernicus) believed that the planets' orbits were perfectly circular with the Sun at the center. Kepler corrected this, and **Kepler's first law** states that the planetary orbits are ellipses with the Sun lying at a focal point.

Now we will determine the period τ of a bounded elliptic orbit. Integrating Kepler's second law (3.2) over one orbit and recalling the area of an ellipse, we have

$$\pi ab = S = \tfrac{1}{2}L\tau.$$

This yields the explicit formula

$$\tau = 2\pi m\tfrac{ab}{L} = \pi k\sqrt{\tfrac{m}{2|E|^3}}$$

for the period as a function of the energy. Using the formula (3.14) for the semi-major axis a in terms of the energy E, we obtain

$$\tau = 2\pi\sqrt{\tfrac{ma^3}{k}}. \tag{3.15}$$

This demonstrates **Kepler's third law**: the period τ of a planet's orbit is proportional to $a^{3/2}$, where a is the semi-major axis.

In practice we know that the mass (or charge) sitting at the origin is not perfectly stationary, but instead is perturbed by the particle's presence. We will now remedy this. The two-body problem seeks the motion for a closed system consisting of two gravitational bodies with positions $\mathbf{x}_i$ and masses m_i, for $i = 1, 2$. The system is conservative with potential

$$V(\mathbf{x}_1, \mathbf{x}_2) = -\frac{Gm_1m_2}{|\mathbf{x}_1 - \mathbf{x}_2|}, \tag{3.16}$$

where G is the gravitational constant.

By Newton's first law (cf. Proposition 1.15) we know that the center of mass moves with constant velocity. We choose a reference frame so that the center of mass lies at the origin:

$$m_1\mathbf{x}_1 + m_2\mathbf{x}_2 \equiv 0.$$

Let $\mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2$ denote the distance between the particles. We can recover the positions from $\mathbf{x}$ via

$$\mathbf{x}_1 = \tfrac{m_2}{m_1+m_2}\mathbf{x}, \qquad \mathbf{x}_2 = -\tfrac{m_1}{m_1+m_2}\mathbf{x}. \tag{3.17}$$

The total energy can be written solely in terms of $\mathbf{x}$ as

$$E = \tfrac{1}{2}m_1|\dot{\mathbf{x}}_1|^2 + \tfrac{1}{2}m_2|\dot{\mathbf{x}}_2|^2 + V(|\mathbf{x}_1 - \mathbf{x}_2|) = \tfrac{1}{2}\mu|\dot{\mathbf{x}}|^2 + V(|\mathbf{x}|), \tag{3.18}$$

where $\mu = m_1m_2/(m_1 + m_2)$ is the **reduced mass**. In other words, the two-body system is equivalent to a single-particle of mass μ moving in the external central field $V(|\mathbf{x}|)$. Solving for the motion of $\mathbf{x}$ in the reduced problem (3.18) yields the solutions to the original problem (3.16) via (3.17). In particular, the motion of two gravitational bodies (or two attractive charges) will be two conic sections with a shared focus at the origin.

3.4. Virial theorem

The virial theorem is a general formula for the long-time average of a system's kinetic energy. In the special case of a single particle in a homogeneous central field, it takes a particularly simple form.

Suppose we have a system of N particles in $\mathbb{R}^d$. The virial theorem is based upon the following simple calculation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\Bigg(\sum_{i=1}^{N}\mathbf{x}_i\cdot\mathbf{p}_i\Bigg) = \sum_{i=1}^{N}\dot{\mathbf{x}}_i\cdot\mathbf{p}_i + \sum_{i=1}^{N}\mathbf{x}_i\cdot\dot{\mathbf{p}}_i = 2K + \sum_{i=1}^{N}\mathbf{F}_i\cdot\mathbf{x}_i. \tag{3.19}$$

We now take the long-time average

$$\langle f\rangle = \lim_{T\to\infty}\frac{1}{T}\int_0^T f(t)\,\mathrm{d}t \tag{3.20}$$

of both sides of (3.19):

$$\left\langle \frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_{i=1}^{N} \mathbf{x}_i \cdot \mathbf{p}_i\right)\right\rangle = 2\langle K\rangle + \left\langle \sum_{i=1}^{N} \mathbf{F}_i \cdot \mathbf{x}_i \right\rangle. \tag{3.21}$$

Note that for any bounded function f we have

$$\left\langle \frac{\mathrm{d}f}{\mathrm{d}t} \right\rangle = \lim_{T\to\infty} \frac{f(T) - f(0)}{T} = 0.$$

Therefore, if all particle motion is bounded, then the LHS of (3.21) vanishes. Altogether, we conclude:

Theorem 3.5 (Clausius' virial theorem [Cla70])**.** *If the motion of a Newtonian system of N particles is bounded, then the long-time average (defined by* (3.20)*) of the kinetic energy obeys*

$$-2\langle K\rangle = \left\langle \sum_{i=1}^{N} \mathbf{F}_i \cdot \mathbf{x}_i \right\rangle. \tag{3.22}$$

In particular, for a single particle in a central field with potential V that is homogeneous of degree α we have

$$\langle K\rangle = \tfrac{\alpha}{2}\langle V\rangle. \tag{3.23}$$

Proof. It only remains to prove the special case (3.23). Writing $V(r) = kr^\alpha$ for $k \in \mathbb{R}$ a constant, we have

$$\mathbf{F} \cdot \mathbf{x} = -V'(r)r = -\alpha V(r).$$

Together with (3.22), this yields (3.23). □

The quantity on the RHS of (3.22) is called the **virial**. This name is due to Clausius, and is derived from the Latin word for "force".

Similar to how the conservation of momentum and energy are associated to symmetries, the virial identity (3.23) is connected to a scaling symmetry. Indeed, for a potential V that is homogeneous of degree α, it is straightforward to check that if $\mathbf{x}(t)$ solves Newton's equation (1.3), then so does $\lambda^2\mathbf{x}(\lambda^{\alpha-2}t)$ for any constant $\lambda > 0$.

Example 3.6. For the gravitational potential (3.9) we have $\alpha = -1$, and thus

$$\langle K\rangle = -\tfrac{1}{2}\langle V\rangle.$$

In particular, for circular orbits the potential $V = -kr^{-1}$ is constant, and so we deduce that the velocity v is proportional to $r^{-1/2}$. On the other hand, the period τ is given by $2\pi r/v$ and thus is proportional to $r^{3/2}$; this agrees with Kepler's third law (3.15).

The version (3.22) of the virial theorem is commonly used in physical applications. Mathematically however, the computation (3.19) is arguably equally as important, particularly in deriving monotonicity formulas.

Example 3.7. Consider a single particle moving in a central field in $\mathbb{R}^3$ with potential V, and suppose that the potential is repulsive in the sense that the radial component of the force always points away from the origin:

$$\mathbf{x} \cdot \nabla V(\mathbf{x}) < 0 \quad \text{for all } \mathbf{x} \neq 0. \tag{3.24}$$

From (3.19) we see that

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{x} \cdot \mathbf{p}) \geq 2K > 0,$$

and thus $\mathbf{x} \cdot \mathbf{p}$ is a strictly increasing function of time along any trajectory; in particular, there can be no closed orbits for the system. Equivalently, we can phrase this in terms of its antiderivative $\frac{m}{2}|\mathbf{x}(t)|^2$:

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\big(|\mathbf{x}(t)|^2\big) \geq \tfrac{4}{m}K > 0,$$

from which we see that $|\mathbf{x}(t)|^2$ is a strictly convex function.

Example 3.8 (Morawetz inequality [Tao06, Ex. 1.32])**.** Alternatively, it is also common to work in terms of the function $|\mathbf{x}(t)|$. Consider the system in the previous example. For $\mathbf{x} \neq 0$ we compute

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\,|\mathbf{x}(t)| = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathbf{x}}{|\mathbf{x}|}\cdot\dot{\mathbf{x}}\right) = \frac{|\dot{\mathbf{x}}|^2}{|\mathbf{x}|} - \frac{(\mathbf{x}\cdot\dot{\mathbf{x}})^2}{|\mathbf{x}|^3} + \frac{\mathbf{x}}{|\mathbf{x}|}\cdot\ddot{\mathbf{x}} = \frac{|\pi_{\mathbf{x}}(\dot{\mathbf{x}})|^2}{|\mathbf{x}|} - \frac{\mathbf{x}\cdot\nabla V}{m|\mathbf{x}|}, \tag{3.25}$$

where

$$\pi_{\mathbf{x}}(\mathbf{v}) = \mathbf{v} - \frac{\mathbf{x}}{|\mathbf{x}|}\left(\frac{\mathbf{x}}{|\mathbf{x}|}\cdot\mathbf{v}\right)$$

denotes the component of $\mathbf{v}$ perpendicular to $\mathbf{x}$. For a repulsive potential V (in the sense of (3.24)), we obtain

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\,|\mathbf{x}(t)| \geq \frac{|\pi_{\mathbf{x}}(\dot{x})|^2}{|\mathbf{x}|} > 0.$$

Consequently $|\mathbf{x}(t)|$ is strictly convex, or equivalently $\frac{\mathbf{x}}{|\mathbf{x}|}\cdot\dot{\mathbf{x}}$ is strictly increasing. Physically, this tells us that a particle initially moving towards the origin is slowing down, and a particle moving away from the origin cannot reverse direction.

If the potential V is also nonnegative, then we have

$$\tfrac{1}{2}m|\dot{x}|^2 \leq E_0$$

where E_0 is the initial total energy, and thus

$$\left|\frac{\mathbf{x}}{|\mathbf{x}|}\cdot\dot{\mathbf{x}}\right| \leq |\dot{\mathbf{x}}| \leq \sqrt{\tfrac{2}{m}E_0}.$$

Integrating (3.25) in time we then obtain

$$\int_{-\infty}^{\infty} \frac{|\pi_{\mathbf{x}(t)}(\dot{\mathbf{x}}(t))|^2}{|\mathbf{x}(t)|}\,\mathrm{d}t \leq 2\sqrt{\tfrac{2}{m}E_0} \tag{3.26}$$

(provided that $\mathbf{x}(t)$ exists for all $t \in \mathbb{R}$ and is nonvanishing). Physically, this tells us that the angular component of the velocity is decaying in time and the motion becomes predominantly radial.

The estimate (3.26) is an example of a **Morawetz inequality**, and such inequalities have played an important role in the context of PDEs. They are named after Morawetz's pioneering work on the scattering problem for the linear wave equation with an obstacle; see [Mor75, LP89] for details. More recently, Morawetz inequalities have also proven to be a powerful tool in the study of nonlinear PDEs.

For more examples of monotonicity formulas in the context of Newtonian systems, see [Tao06, §1.5]. For an introduction to monotonicity formulas for PDEs, see [KV13, §7] and [Tao06, Ch. 2-3].

3.5. Exercises

3.1. Consider the central field with potential

$$V(r) = -kr^{-2}$$

for $k > 0$ a constant. Show that trajectories with negative energy reach the origin in finite time by considering the effective potential.

3.2 (Method of similarity)**.** Suppose that the potential energy of a central field is a homogeneous function of degree α:

$$V(r) = kr^{\alpha}$$

for $k \in \mathbb{R}$ a constant. Show that if a curve γ is a trajectory, then the rescaled curve $\lambda\gamma$ for any constant $\lambda > 0$ is also a trajectory. For a periodic trajectory γ, determine the ratio of the periods of these trajectories. Conclude that the period is constant for the harmonic oscillator ($\alpha = 2$), and that the gravitational potential ($\alpha = -1$) obeys Kepler's third law.

3.3 (Escape velocity)**.** Let r_0 denote the radius of the Earth, and g the gravitational acceleration at the Earth's surface. The gravitational potential energy of the Earth is

$$V(r) = -\tfrac{gr_0^2}{r}.$$

Determine the escape velocity, i.e. the minimum velocity a particle must be given on the surface of the Earth in order for it to travel infinitely far away.

3.4 (Cosmic velocities)**.** Consider the gravitational potential energy of the Earth as in the previous problem. The escape velocity v_2 is sometimes called the second cosmic velocity. The first cosmic velocity is the speed of a particle in a circular orbit with radius equal to that of the Earth. Find the first cosmic velocity v_1 and show that $v_2 = \sqrt{2}v_1$.

3.5 (Geosynchronous orbit [Nah16])**.** It is useful for communication satellites to be in geosynchronous orbit, so that their orbital period is one day and the satellite appears to hover in the sky. We will calculate the height of this orbit for Earth in two different ways.

(a) Let m be the satellite's mass, $M = 5.98 \times 10^{24}\,\text{kg}$ be the Earth's mass, v be the satellite's velocity, and R_s the radius of the satellite's circular orbit. Determine R_s by equating the gravitational and centripetal accelerations of a circular orbit and writing $v = 2\pi R_s/T$ where T is the length of a day.

(b) Use Kepler's third law to calculate the same value for R_s.

3.6 (Satellite paradox [Nah16])**.** Satellites in low Earth orbit experience significant atmospheric drag, which actually increases the speed of the satellite.

(a) For a circularly orbiting satellite in Earth's gravitational potential, conclude from the virial theorem that the satellite's total energy is

$$E = -\tfrac{1}{2}mv^2.$$

Alternatively, this relation can be obtained by equating the gravitational and centripetal accelerations, solving for v, and substituting v into the kinetic energy.

(b) Differentiate the result from part (a) to determine $\dot{v}$ in terms of $\dot{E}$. Assuming the energy loss rate (i.e. dissipated power) of the satellite is

$$\dot{E} = -cv$$

for $c > 0$ a constant, show that $\dot{v} > 0$.

3.7 (Solar and lunar tides [Nah16])**.** The gravitational force between two bodies of masses m_1 and m_2 has magnitude

$$F(r) = Gm_1m_2r^{-2},$$

where r is the distance between the bodies' centers and G is the universal gravitational constant. For the Earth, Sun, and Moon, we have

$$\begin{aligned} M_s &= \text{mass of the Sun} = 2 \times 10^{30}\,\text{kg}, \\ M_m &= \text{mass of the Moon} = 7.35 \times 10^{22}\,\text{kg}, \\ R_s &= \text{Earth-Sun separation} = 93 \times 10^6 \text{ miles}, \\ R_m &= \text{Earth-Moon separation} = 2.39 \times 10^5 \text{ miles}. \end{aligned}$$

(a) Find the ratio of the Sun's and the Moon's gravitational forces on the Earth. Even though the Sun is much farther from the Earth, the Sun's gravitational force on the Earth is much greater than the Moon's.

(b) As the Earth is not a point mass, then the Sun's gravitational force is stronger (weaker) on the side of the Earth closest (farthest) from the Sun. This causes water to bulge at the points closest and furthest from the Sun, which is called the solar high tides. Calculate the maximum difference in gravitational force in terms of Earth's radius R for both the Sun and the Moon.

(c) Extract the leading term in the limit $R/R_s \ll 1$ and $R/R_m \ll 1$ for each expression in part (b). Calculate their ratio and conclude that, although the Sun's gravitational force is stronger, the lunar tides are more than twice as large as the solar tides.

3.8 (Energy of the ocean tides [Nah16])**.** The lunar tides are not directly in line with the centers of the Earth and Moon, but are rather carried ahead slightly by the Earth's rotation and friction. This means that the Moon's gravitational pull on both tides produce torque. The Moon's pull on the farther tide increases the Earth's rotational speed, but the stronger pull on the nearer tide is counter-rotational, and so the overall effect decreases the Earth's rotational speed. Atomic clocks have measured that the length of a day is increasing at the rate of about 2 milliseconds per century.

(a) Let Ω denote the angular rotation rate of the Earth and let T denote the length of a day in seconds, so that $\Omega T = 2\pi$. By integrating the kinetic energy over the volume of the Earth, show that the rotational energy E is given by

$$E = \tfrac{1}{2}\Omega^2 I,$$

where

$$I = \int_{r\le R} (x^2 + y^2)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$$

is the moment of inertia.

(b) Show that for a solid sphere of radius R and constant mass density ρ the moment of inertia is

$$I = \tfrac{8\pi}{15} R^3 \rho,$$

or in terms of the total mass M,

$$I = \tfrac{2}{5} M R^2.$$

The Earth is not a constant-density sphere, and so rather than $\frac{2}{5}$ the coefficient is approximately 0.3444.

(c) Write the rotational energy E as a function of the period τ, and show that

$$\frac{\mathrm{d}E}{\mathrm{d}\tau} = -\frac{4 \times 0.3444 \times M\pi^2 R^2}{T^3}.$$

Taking τ to be the length of a day, $\Delta\tau$ to be 2 milliseconds, $M = 5.98 \times 10^{24}$ kg, and $R = 6.38 \times 10^6$ m, find the change in the Earth's rotational energy ΔE over a century. Dividing ΔE by the number of seconds in a century, conclude that the power of the ocean tides is $3,260$ gigawatts (which is 4.37 billion horsepower).

3.9 (Moon recession rate [Nah16])**.** As in Exercise 3.8, tidal friction decreases the Earth's rotational angular momentum. Consequently, the Moon's orbital angular momentum increases in order to conserve total angular momentum, which results in the Moon drifting away from the Earth. We will estimate this recession rate, assuming that all of the momentum is transferred to the Moon's orbit (rather than its rotation).

(a) Consider the Moon as a point mass m orbiting circularly about the Earth at a radius r, with speed v and angular speed ω radians per second. What is the magnitude L_m of Moon's orbital angular momentum about the Earth?

(b) The gravitational force on the Moon by the Earth has magnitude

$$F = GMmr^{-2},$$

where M is the mass of the Earth and G is the universal gravitational constant. Equating the gravitational and centripetal accelerations of the Moon, find v as a function of r. Use this to determine the angular momentum L_m as a function of r.

(c) From part (b) of Exercise 3.8, the rotational angular momentum of the Earth is $L_e = 0.3444\, MR^2\Omega$ where Ω is Earth's rotation rate. Expressing Ω in terms of the day length T in seconds, find L_e as a function of T and calculate $\frac{\mathrm{d}L_e}{\mathrm{d}T}$.

(d) Using the daily change $\Delta T = 2 \times 10^{-5}/365$ seconds in the length of a day, approximate the daily change and the yearly change in ΔL_e.

(e) Equating change in the Moon's orbital momentum ΔL_m with the change in Earth's rotational momentum $|\Delta L_e|$, find the yearly change in the Moon's orbital radius. Using the values

$$\begin{aligned}
M &= \text{mass of the Earth} = 5.98 \times 10^{24}\,\text{kg},\\
m &= \text{mass of the Moon} = 7.35 \times 10^{22}\,\text{kg},\\
r &= \text{radius of Moon's orbit} = 3.84 \times 10^{8}\,\text{m},\\
R &= \text{radius of the Earth} = 6.37 \times 10^{6}\,\text{m},\\
G &= \text{gravitational constant} = 6.67 \times 10^{-11}\,\text{m}^3\,\text{kg}^{-1}\,\text{s}^{-2},
\end{aligned}$$

conclude that the Moon is receding from the Earth at a rate of 3.75 centimeters (or 1.48 inches) per year. This value is in outstanding agreement with measurements made by a laser on Earth and corner cube reflectors on the Moon.

3.10. Consider the central field with potential

$$V(r) = -kr^{-2}$$

for $k > 0$ a constant. Show that

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\big(|\mathbf{x}(t)|^2\big) = \tfrac{4}{m}E,$$

where E is the total energy. Conclude that trajectories with negative energy reach the origin in finite time.

3.11 (Central field scattering)**.** In this problem we consider a classical model for a beam of charged particles passing near a repulsive central charge. Consider a repulsive central field in $\mathbb{R}^3$ that tends to zero as $|\mathbf{x}| \to \infty$. Suppose we have a uniform beam of particles all of the same mass and energy whose motion begins and ends colinearly at infinity. The intenstiy I of the beam is the number of particles crossing unit area normal to the initial direction of travel per unit time.

(a) Define the impact parameter s for a particle of mass m and initial velocity v_0 via

$$L = mv_0 s = s\sqrt{2mE}.$$

Using the facts from section 3.1, show that for the solid angle $\Omega \subset S^2$ the scattering cross section $\sigma(\Omega)$—the number of particles scattered per unit solid angle per unit time divided by the incident intensity—is given by

$$\sigma(\Theta) = -\frac{s}{\sin\Theta}\frac{\mathrm{d}s}{\mathrm{d}\Theta},$$

where Θ is the angle between the incident and scattered beams.

(b) Suppose the incident particles have charge $-q < 0$ and the fixed particle has charge $-Q < 0$. The motion is dictated by the Coulomb force

$$\mathbf{F}(r) = qQr^{-2}\hat{\mathbf{r}} = \nabla V, \qquad V(r) = qQr^{-1}.$$

Although we assumed that $V = -kr^{-1}$ with $k > 0$ in section 3.3 in order to model celestial motion, we never needed that k is positive, and so the explicit solutions are still valid. By relating the total angle of deflection Θ to the eccentricity ϵ of the hyperbolic trajectories, show that

$$\sin\tfrac{\Theta}{2} = \tfrac{1}{\epsilon}, \qquad \cot\tfrac{\Theta}{2} = \tfrac{2Es}{qQ}.$$

Using the previous part, conclude that

$$\sigma(\Theta) = \big(\tfrac{qQ}{4E}\big)^2\big(\sin\tfrac{\Theta}{2}\big)^{-4}.$$

This is the Rutherford scattering cross section. As a classical approximation of a quantum system, it has some limitations. For example, if we were to integrate this expression over the sphere we would obtain an infinite total scattering cross section, which is of course impossible.

(c) As with Kepler's problem, the central charge is not truly fixed but instead recoils as a result of the scattering. Assume the central particle is initially stationary. Let the subscript 1 refer to the scattered particle, primed coordinates denote coordinates relative to the center of mass, and $\mathbf{X}$ represent the position of the center of mass in laboratory coordinates so that $\mathbf{x}_1 = \mathbf{X} + \mathbf{x}_1'$, $\mathbf{v}_1 = \dot{\mathbf{x}}_1 = \dot{\mathbf{X}} + \mathbf{v}_1'$. To replace the angle Θ between the initial and final vectors between the charges, consider the deflection angle θ between the initial and final directions of the scattered particles. Use the conservation of total momentum to show that

$$\tan\theta = \frac{|\mathbf{v}_1'|\sin\Theta}{|\mathbf{v}_1'|\cos\Theta + |\dot{\mathbf{X}}|}.$$

Then by considering the initial relative velocity, show that

$$\tan\theta = \frac{\sin\Theta}{\cos\Theta + \frac{m_1}{m_2}}.$$

As we would expect experimentally, when $m_2 \gg m_1$ the initially stationary particle does not experience significant recoil and $\theta \approx \Theta$.

(d) The number of particles scattered into a fixed element of solid angle must be the same in both the laboratory and center-of-mass coordinates. Consequently, show that the cross section $\sigma'(\theta)$ in the laboratory system is given by

$$\sigma'(\theta) = \sigma(\Theta)\frac{\sin\Theta}{\sin\theta}\frac{\mathrm{d}\Theta}{\mathrm{d}\theta} = \sigma(\Theta)\frac{\mathrm{d}(\cos\Theta)}{\mathrm{d}(\cos\theta)}.$$

(e) Rutherford was interested in α-particle scattering, for which corrections to $m_1/m_2 = 1$ are negligible. When $m_1 = m_2$, show that $\theta = \frac{1}{2}\Theta$; in particular, $0 \le \theta \le \pi/2$ and there can be no back scattering. Conclude

$$\sigma'(\theta) = 4\cos\theta\,\sigma(2\theta)\ , \qquad \frac{|\mathbf{v}_1|}{|\mathbf{v}_0|} = \cos\theta.$$

PART II

LAGRANGIAN MECHANICS

The Lagrangian perspective is based upon the principle of least action, which is a coordinate-free reformulation of mechanics on configuration space (and its tangent bundle). Unpacking the principle of least action yields the Euler–Lagrange equations of motion—a system with one second order differential equation for each degree of freedom—and showcases some fundamental ideas from the calculus of variations. The coordinate-independence allows us to work with any choice of coordinates or on any manifold. In particular, when the coordinates are chosen to align with symmetries of the system, the Euler–Lagrange equations are effective in identifying the corresponding conserved quantities, reducing the number of equations, and simplifying the system.

CHAPTER 4

EULER–LAGRANGE EQUATIONS

We will reformulate Newton's equations as the principle of least action. Unpacking this axiom to obtain the Euler–Lagrange equations of motion will feature some fundamental ideas from the calculus of variations. This presentation of the calculus of variations follows [AKN06, Ch. 1], and in the rest of the material is based on [LL76, Ch. 1–2], [Arn89, Ch. 3], and [Gol51, Ch. 1–2].

4.1. Principle of least action

For a mechanical system with N particles, we replace the configuration space $(\mathbb{R}^d)^N$ by a smooth manifold M. While physics texts often focus on the derivation for Euclidean space, we will present the theory for general manifolds. This level of generality is not superfluous; indeed, the freedom in the choice of configuration space and coordinates is a powerful feature of Lagrangian mechanics. (Familiarity with manifolds is not strictly necessary however, because mathematical statements for manifolds will often be easily reducible to that of Euclidean space; cf. Proposition 4.5.)

We will use q to denote any (local) coordinates on M (sometimes called **generalized coordinates** in physics), and v (often $\dot{q}$ in physics) to denote a tangent vector in the tangent space T_qM at q. The number of components $n := \dim M$ of q is called the **degrees of freedom** of the system.

Definition 4.1. A **Lagrangian system** $(M, \mathscr{L})$ is a smooth n-dimensional manifold M called the **configuration space** together with a smooth function $\mathscr{L}(t, q, v) : I \times TM \to \mathbb{R}$ called the **Lagrangian**, where TM is the tangent bundle of M and $I \subset \mathbb{R}$ is an interval.

As we will see in section 4.2, the following abstract statement encodes Newton's equations:

Definition 4.2 (Hamilton's principle of least action)**.** A smooth curve $q(t)$ from $[0, T]$ into M is a **motion** of the Lagrangian system $(M, \mathscr{L})$ if it is a critical point of the **action** functional

$$S(q(t)) = \int_0^T \mathscr{L}(t, q(t), \dot{q}(t))\,\mathrm{d}t. \tag{4.1}$$

The principle of least action often bears Hamilton's name, but it was also independently discovered by Jacobi.

In this section, we will see how to extract equations of motion from the principle of least action. The principle is called "least" action because it turns out that the motion is often a minimum; however, we will not make use of this additional assumption.

The goal of the calculus of variations is to find the extrema of functionals. A **path** from $a_0 \in M$ to $a_1 \in M$ (not necessarily distinct) starting at time 0 and ending at time $T > 0$ is a smooth map $\gamma : [0, T] \to M$ with $\gamma(0) = a_0$ and $\gamma(T) = a_1$. Let Ω denote the collection of all such paths. A **functional** is a function Φ from Ω into $\mathbb{R}$.

Example 4.3. The arc length of the graph of $\mathbf{x}(t)$ from $[0, T]$ into $M = \mathbb{R}^n$ is a functional. It takes as input a smooth function $\mathbf{x} : [0, T] \to \mathbb{R}^n$ and returns the value

$$\Phi(\mathbf{x}(t)) = \int_0^T \sqrt{1 + \dot{\mathbf{x}}^2}\, \mathrm{d}t.$$

Intuitively, we expect the path of minimum length between two points to be the line segment connecting those two points. Indeed, by the fundamental theorem of calculus we have

$$\big|(T, a_1) - (0, a_0)\big| = \left| \int_0^T (1, \dot{\mathbf{x}})\, \mathrm{d}t \right| \leq \int_0^T |(1, \dot{\mathbf{x}})|\, \mathrm{d}t = \int_0^T \sqrt{1 + |\dot{\mathbf{x}}|^2}\, \mathrm{d}t,$$

with equality if and only if $\dot{\mathbf{x}}$ is constant. The more systematic machinery that we develop in this section should also return this answer.

In order to solve for the optimizer, we want to obtain an equation that must be satisfied by the extremum of our functional. From calculus we expect that the first derivative should vanish at an extremum, and so we want to define a notion of first derivative for functionals. For more concrete examples we do not need to assume arbitrary smoothness (cf. Exercise 4.2) or even that an extremum exists *a priori* (cf. Exercise 4.5), but for clarity we will assume the extremum exists and that everything is smooth.

A (**fixed-endpoint**) **variation** of a path $\gamma \in \Omega$ is a smooth map $H(s, t) = H_s(t)$ from $(-\epsilon, \epsilon) \times [0, T]$ to M for some $\epsilon > 0$ such that:

- $H_0 = \gamma$,
- $H_s \in \Omega$ for all $s \in (-\epsilon, \epsilon)$, and
- $H(s, t_i) = a_i$ for $i = 0, 1$ for all $s \in (-\epsilon, \epsilon)$.

In other words, the paths H_s for various s form a smooth deformation of γ, which is equal to γ at $s = 0$ and always connect a_1 to a_2 for other values of s.

In analogy with calculus on Euclidean space, we will call a functional Φ **differentiable** at a path $\gamma \in \Omega$ with **derivative** (or **first variation**) $\mathrm{d}\Phi|_\gamma$ (or $\delta\Phi$) if the limit

$$\mathrm{d}\Phi|_\gamma \left(\frac{\partial H_s}{\partial s} \right) = \lim_{s \to 0} \frac{\Phi(H_s) - \Phi(\gamma)}{s}$$

exists for all variations H of γ. In other words, there should exist a function $\mathrm{d}\Phi|_\gamma$ so that the Taylor expansion

$$\Phi(H_s) = \Phi(\gamma) + s\,\mathrm{d}\Phi|_\gamma\left(\frac{\partial H_s}{\partial s}\right) + o(s)$$

holds. We expect the function $\mathrm{d}\Phi|_\gamma$ will be linear in $\frac{\partial H_s}{\partial s}$ (like $\mathbf{v} \mapsto \nabla f(\mathbf{x}_0)\cdot\mathbf{v}$ on Euclidean space). We need Φ to be a function of $\frac{\partial H_s}{\partial s}$ instead of H because the space of derivatives $\frac{\partial H_s}{\partial s}$ will be linear, unlike the space of variations H which will be nonlinear if M is not flat.

It remains to define $\mathrm{d}\Phi|_\gamma$ and $\frac{\partial H_s}{\partial s}$. These are technical details that do not appear in the Euclidean theory, but we present them for the sake of the general manifold theory. We can think of Ω as a manifold (albeit infinite-dimensional), and a variation as a path on Ω through γ at $s = 0$. The derivative $\frac{\partial H_s}{\partial s}$ should be tangent to Ω at the path H_s. We define a tangent vector W to Ω at a path $\gamma \in \Omega$ to be a function which associates to each $t \in [0,T]$ a tangent vector $W_t \in T_{\gamma(t)}M$, and is smooth in the sense that for every smooth function $f : M \to \mathbb{R}$ the function $t \mapsto \mathrm{d}f(W_t) \in \mathbb{R}$ is smooth. The tangent space $T_\gamma\Omega$ is the space of all tangent vectors W at γ such that $W_0 = 0 = W_T$. Now we can define the tangent vector $\frac{\partial H_s}{\partial s}(0)$ to the variation H_s at $s = 0$ to be the set of derivatives

$$\frac{\partial H}{\partial s}(0,t) \in T_{\gamma(t)}M \quad \text{for } t \in [0,T].$$

As

$$\frac{\partial H}{\partial s}(0,t_0) = 0 \quad \text{and} \quad \frac{\partial H}{\partial s}(0,t_1) = 0$$

by the fixed-endpoint requirement, then we indeed have $\frac{\partial H_s}{\partial s}(0) \in T_\gamma\Omega$. Now we define

$$\mathrm{d}\Phi|_\gamma\left(\frac{\partial H_s}{\partial s}\right) = \frac{\mathrm{d}}{\mathrm{d}s}\Phi \circ H_s\Big|_{s=0}.$$

One can check that $\mathrm{d}\Phi|_\gamma$ is well-defined and linear as expected (cf. Exercise 4.1).

Example 4.4. Consider the arc-length functional Φ of Example 4.3. Given two points $\mathbf{a}_0, \mathbf{a}_1 \in \mathbb{R}^n$, the space Ω of paths from $\mathbf{a}_0$ to $\mathbf{a}_1$ is the set of smooth functions $[0,T] \to \mathbb{R}^n$ with $\mathbf{x}(t_i) = \mathbf{a}_i$ for $i = 0, 1$. For any path $\mathbf{x} : [0,T] \to \mathbb{R}^n$, a variation $H_s(t)$ of $\mathbf{x}$ takes the form $\mathbf{x}(t) + \mathbf{h}_s(t)$, where $\mathbf{h}_s : [0,T] \to \mathbb{R}^n$ is smooth satisfying $\mathbf{h}_s(0) = 0 = \mathbf{h}_s(T)$ for all $s \in (-\epsilon, \epsilon)$ and $\mathbf{h}_0(t) \equiv 0$.

The derivative $\frac{\partial H}{\partial s}$ is equal to $\frac{\partial \mathbf{h}_s}{\partial s}(t)$. As $\mathbf{h}_0(t) \equiv 0$, then the variation at $s = 0$ is equal to $\mathbf{x}(t)$, and so $\frac{\partial H}{\partial s}(0,t) = \frac{\partial \mathbf{h}_0}{\partial s}(t)$ is a vector centered at $\mathbf{x}(t)$ and pointing in the direction of the variation $\mathbf{h}_s(t)$ for small s. Moreover, $\frac{\partial H}{\partial s}(0,t_i) = \frac{\partial \mathbf{h}_0}{\partial s}(t_i) = 0$ for $i = 1, 2$ since $\mathbf{h}_s(0) = 0 = \mathbf{h}_s(T)$ for all $s \in (-\epsilon, \epsilon)$.

A tangent vector W to Ω at $\mathbf{x}(t)$ is a set of vectors $\{\mathbf{w}_t : t \in [0,T]\}$ such that $\mathbf{w}_t$ is centered at $\mathbf{x}(t)$, the vectors $\mathbf{w}_0$ and $\mathbf{w}_T$ at the endpoints vanish, and $\mathbf{w}_t$ depends smoothly on t (in the sense that $t \mapsto \mathbf{v}\cdot\mathbf{w}_t$ is smooth, or equivalently every component of $\mathbf{w}_t$ is a smooth function of t).

For the rest of this section, we will restrict our attention to the action functional S defined in (4.1). If we take $\mathscr{L}(t, \mathbf{x}, \mathbf{y}) = \sqrt{1 + |\mathbf{y}|^2}$, we recover the functional of Example 4.3. The reason we insisted that $\mathscr{L}$ be differentiable is so that the action is differentiable. To study the consequences of the principle of least action, we seek a **critical point** γ for Φ, that is a path γ that satisfies $\mathrm{d}\Phi|_\gamma \equiv 0$.

Proposition 4.5 (Euler–Lagrange equations)**.** *The action functional* (4.1) *is differentiable, with derivative*

$$\mathrm{d}S|_\gamma\left(\frac{\partial H_s}{\partial s}\right) = \int_0^T \left(\frac{\partial \mathscr{L}}{\partial q} - \frac{d}{dt}\frac{\partial \mathscr{L}}{\partial \dot{q}}\right) \cdot \frac{\partial H_s}{\partial s}\, dt. \tag{4.2}$$

Consequently, a path $q(t)$ is a critical point for the action if and only if $q(t)$ solves

$$\frac{d}{dt}\left[\frac{\partial \mathscr{L}}{\partial \dot{q}}\big(t, q(t), \dot{q}(t)\big)\right] - \frac{\partial \mathscr{L}}{\partial q}\big(t, q(t), \dot{q}(t)\big) = 0. \tag{4.3}$$

The n-many second-order differential equations (4.3) are called the **Euler–Lagrange equations** for the functional S, or simply the **Lagrange equations** when applied to a mechanical system. Note that (4.3) must hold for any choice of coordinates q, where $\frac{\partial \mathscr{L}}{\partial q}$ is the gradient of $\mathscr{L}(t, q, v)$ in the q variables. The derivative $\frac{\partial \mathscr{L}}{\partial \dot{q}}$ is a convenient notation for the derivative of the Lagrangian $\mathscr{L}(t, q, v)$ in the velocity variables v, and should technically be notated as $\frac{\partial \mathscr{L}}{\partial v}(t, q, \dot{q})$. Although (4.3) is often shortened to

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}} - \frac{\partial \mathscr{L}}{\partial q} = 0,$$

we are meant to plug in q and $\dot{q}$ before taking the total time derivative $\frac{\mathrm{d}}{\mathrm{d}t}$, which for example will turn $\dot{q}$ into $\ddot{q}$.

Proof. Fix a set of coordinates q on M, let γ be a path, and let H be a variation of γ. By taking the variation of γ to be supported within the image of the coordinate patch q and shrinking the interval $[0, T]$ if necessary, we will work solely within the domain of q in $\mathbb{R}^n$. Let $\mathbf{x}(t)$ denote the path in $\mathbb{R}^n$, $\mathscr{L}(t, \mathbf{x}, \dot{\mathbf{x}})$ denote the Lagrangian in $\mathbb{R}^n$, and $\mathbf{x}(t) + \mathbf{h}(t)$ the variation $H_s(t)$ in $\mathbb{R}^n$ (where the s-dependence of $\mathbf{h}$ is suppressed). Note that the fixed endpoint condition requires that $\mathbf{h}(0) = 0 = \mathbf{h}(T)$.

Now that we may work in Euclidean space, we can now use the key idea that lies at the heart of the Euler–Lagrange theory. As $\mathscr{L}$ is differentiable, we may Taylor expand and write

$$\mathscr{L}(t, \mathbf{x}+\mathbf{h}, \dot{\mathbf{x}}+\dot{\mathbf{h}}) = \mathscr{L}(t, \mathbf{x}, \dot{\mathbf{x}}) + \frac{\partial \mathscr{L}}{\partial \mathbf{x}}(t, \mathbf{x}, \dot{\mathbf{x}}) \cdot \mathbf{h}(t) + \frac{\partial \mathscr{L}}{\partial \dot{\mathbf{x}}}(t, \mathbf{x}, \dot{\mathbf{x}}) \cdot \dot{\mathbf{h}}(t) + \mathcal{O}(|\mathbf{h}(t)|^2).$$

Therefore,

$$S(\gamma + \mathbf{h}) - S(\gamma) = \int_0^T \left[\mathscr{L}(t, \mathbf{x} + \mathbf{h}, \dot{\mathbf{x}} + \dot{\mathbf{h}}) - \mathscr{L}(t, \mathbf{x}, \dot{\mathbf{x}})\right] \mathrm{d}t$$
$$= \int_0^T \left(\frac{\partial \mathscr{L}}{\partial \mathbf{x}}(t, \mathbf{x}, \dot{\mathbf{x}}) \cdot \mathbf{h}(t) + \frac{\partial \mathscr{L}}{\partial \dot{\mathbf{x}}}(t, \mathbf{x}, \dot{\mathbf{x}}) \cdot \dot{\mathbf{h}}(t)\right) \mathrm{d}t + \mathcal{O}(|\mathbf{h}|^2).$$

We pulled the term $\mathcal{O}(|\mathbf{h}(t)|^2)$ outside of the integral to get a term $\mathcal{O}(|\mathbf{h}|^2)$ which is bounded by maximum of $|\mathbf{h}(t)|^2$ because $\mathscr{L}$ is continuously differentiable. The integral in the rightmost expression will be the derivative $\mathrm{d}S|_\gamma$. Integrating by parts yields

$$\int_0^T \frac{\partial \mathscr{L}}{\partial \dot{\mathbf{x}}} \cdot \dot{\mathbf{h}} \, \mathrm{d}t = -\int_0^T \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathscr{L}}{\partial \dot{\mathbf{x}}}\right) \cdot \mathbf{h} \, \mathrm{d}t + \left(\frac{\partial \mathscr{L}}{\partial \dot{\mathbf{x}}} \cdot \mathbf{h}\right)\Bigg|_0^T.$$

As $\mathbf{h}(0) = 0 = \mathbf{h}(T)$ the second term on the RHS above must vanish, and inserting this back into the expression for $\mathrm{d}S|_\gamma$ yields (4.2) as desired.

It is clear from the formula (4.2) for $\mathrm{d}S|_\gamma$ that if (4.3) is satisfied then $\mathrm{d}S|_\gamma \equiv 0$. Conversely, assuming that $\mathrm{d}S|_\gamma = 0$ for any variation, we obtain

$$\int_0^T \left(\frac{\partial \mathscr{L}}{\partial \mathbf{x}} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{\mathbf{x}}}\right) \cdot \mathbf{h} \, \mathrm{d}t = 0$$

for all smooth $\mathbf{h} : [0, T] \to \mathbb{R}^n$ with $\mathbf{h}(0) = 0 = \mathbf{h}(T)$. We conclude that the integrand without $\mathbf{h}$ vanishes identically, since otherwise we could pick $\mathbf{h}(t)$ to be a bump function that witnesses any nonzero value and obtain $\mathrm{d}S|_\gamma(\mathbf{h}) \neq 0$. □

In the proof of Proposition 4.5, we only need that the coordinates q are spanning (and not necessarily independent) in order to have enough directions $\mathbf{h}(t)$ to conclude that the Euler–Lagrange equation holds. Therefore, there is no obstruction to extending Proposition 4.5 to more than n coordinates provided that they span the same space.

We also record the following observation:

Corollary 4.6. *Given a Lagrangian $\mathscr{L}(t, q, \dot{q})$, adding a total time derivative:*

$$\widetilde{\mathscr{L}}(t, q, \dot{q}) = \mathscr{L}(t, q, \dot{q}) + \frac{d}{dt}\left[f(t, q)\right]$$

leaves the Euler–Lagrange equations (4.3) *unchanged.*

Proof. The new action is given by

$$\widetilde{S} = \int_0^T \mathscr{L}(t, q, \dot{q}) + \int_0^T \frac{\mathrm{d}f}{\mathrm{d}t} \, \mathrm{d}t = S + f(q(T), T) - f(q(0), 0),$$

and the addition of a constant to S does not affect whether or not a path is a critical point of S. □

Example 4.7. We will apply the Euler–Lagrange equations (4.3) to determine the extrema of the arc length functional of Example 4.3. Using Cartesian coordinates $\mathbf{x}$ on $\mathbb{R}^n$, the Euler–Lagrange equations are

$$0 = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{\mathbf{x}}} - \frac{\partial \mathscr{L}}{\partial \mathbf{x}} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\dot{\mathbf{x}}}{\sqrt{1+|\dot{\mathbf{x}}|^2}}\right) - 0.$$

Integrating once, we see

$$\frac{\dot{\mathbf{x}}}{\sqrt{1+|\dot{\mathbf{x}}|^2}} = \mathbf{a}$$

for some constant $\mathbf{a} \in \mathbb{R}^n$. Squaring shows that the magnitude $|\dot{\mathbf{x}}|$ must be constant, from which we then note that the angle of $\dot{\mathbf{x}}$ must also be constant. Together,

$$\dot{\mathbf{x}} = \mathbf{b}$$

for a new constant $\mathbf{b} \in \mathbb{R}^n$. Finally, integrating yields

$$\mathbf{x}(t) = \mathbf{b}t + \mathbf{c}$$

for $\mathbf{b}, \mathbf{c} \in \mathbb{R}^n$. That is, the extrema of the arc length functional are straight lines. If we had instead chosen, say, polar coordinates, the Euler–Lagrange equations (4.3) would hold for a new Lagrangian $\mathscr{L}$, yielding different differential equations with solutions that still describe straight lines.

4.2. Conservative systems

In section 4.1 we saw how the principle of least action yields the $n = \dim M$ Euler–Lagrange equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}} - \frac{\partial \mathscr{L}}{\partial q} = 0. \tag{4.4}$$

In this section we will see how (4.4) encodes Newton's equations, and thus Newton's principle of determinacy is implied by Hamilton's principle of least action. For this reason, many graduate physics texts opt to begin with the principle of least action and view Newton's equations as a consequence.

Let $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathbb{R}^d$ be Cartesian coordinates on Euclidean space. For a conservative system of N particles, we will see that the right choice of Lagrangian is

$$\mathscr{L}(t, \mathbf{x}, \dot{\mathbf{x}}) = K(\dot{\mathbf{x}}) - V(\mathbf{x}), \tag{4.5}$$

where K and V are the kinetic and potential energies. The principle of least action implies that the motion $\mathbf{x}(t) = (\mathbf{x}_1(t), \ldots, \mathbf{x}_N(t))$ of the system satisfies the Euler–Lagrange equations (4.4). For this Lagrangian, we have

$$\frac{\partial \mathscr{L}}{\partial \dot{\mathbf{x}}} = \frac{\partial K}{\partial \dot{\mathbf{x}}_i} = \frac{\partial}{\partial \dot{\mathbf{x}}}\left(\sum_{i=1}^{N} \tfrac{1}{2} m_i \dot{\mathbf{x}}_i^2\right) = \mathbf{p},$$

$$\frac{\partial \mathscr{L}}{\partial \mathbf{x}} = -\frac{\partial V}{\partial \mathbf{x}} = -\nabla V = \mathbf{F}.$$

Therefore the Euler–Lagrange equations are simply Newton's equations (1.2).

The advantage of the Lagrangian perspective is that we are now no longer restricted to Euclidean space.

Example 4.8. Consider a pendulum consisting of a mass m attached to the end of a rigid massless rod of length ℓ with the other end fixed, allowed to rotate in a vertical plane subject to a constant downward gravitational acceleration g. Let θ denote the angle from the vertical directly below the pivot, which entirely describes the system. The configuration space is the circle S^1, and the Lagrangian is a (time-independent) function defined for $(\theta, \dot{\theta}) \in TS^1 = S^1 \times \mathbb{R}$. The kinetic energy is

$$K = \tfrac{1}{2}mv^2 = \tfrac{1}{2}m\ell^2\dot{\theta}^2,$$

and since the force acting on the mass is $F = ma = -mg\ell\sin\theta$ (cf. Exercise 2.1), then the potential energy is

$$V = -mg\ell\cos\theta.$$

(We picked our integration constant so that $V = 0$ when the mass is at the height of the pivot $\theta = \pi/2$.) The Lagrangian is given by

$$\mathscr{L} = K - V = \tfrac{1}{2}m\ell^2\dot{\theta}^2 + mg\ell\cos\theta,$$

and so the Euler–Lagrange equation is

$$0 = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathscr{L}}{\partial\dot{\theta}} - \frac{\partial\mathscr{L}}{\partial\theta} = m\ell^2\ddot{\theta} + mg\ell\sin\theta \quad \Longrightarrow \quad \ddot{\theta} = -\frac{g}{\ell}\sin\theta,$$

which agrees with what we found using Newton's equation in Exercise 2.1.

We saw that for conservative systems, one good choice for the Lagrangian is (4.5). This choice is not arbitrary, and in fact can be derived from Galileo's principle of relativity (Definition 1.3) applied to the Lagrangian $\mathscr{L}$ rather than the force. Consider a single particle in space whose position is denoted by the Cartesian coordinates $\mathbf{x} \in \mathbb{R}^d$. In an inertial frame, the Lagrangian $\mathscr{L}(t, \mathbf{x}, \dot{\mathbf{x}})$ of this particle cannot be explicitly dependent on position or time by homogeneity, and so $\mathscr{L} \equiv \mathscr{L}(\dot{\mathbf{x}})$. As $\frac{\partial\mathscr{L}}{\partial\mathbf{x}} = 0$, then the Euler–Lagrange equation for this particle is

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathscr{L}}{\partial\dot{\mathbf{x}}} = 0.$$

The quantity $\frac{\partial\mathscr{L}}{\partial\dot{\mathbf{x}}}$ is therefore constant in time, and since $\mathscr{L} \equiv \mathscr{L}(\dot{\mathbf{x}})$ then $\dot{\mathbf{x}}$ must be constant. This is the Lagrangian mechanics proof of Newton's first law (cf. Proposition 1.4): in an inertial frame, the motion of a free particle is uniform in time with constant velocity.

Next, we note that $\mathscr{L}$ cannot depend on the direction of $\dot{\mathbf{x}}$ either since space is isotropic, and so $\mathscr{L} \equiv \mathscr{L}(|\dot{\mathbf{x}}|)$. Let us write this as $\mathscr{L} \equiv \mathscr{L}(|\dot{\mathbf{x}}|^2)$ since we expect $\mathscr{L}$ to be smooth. Let $\mathbf{v} = \dot{\mathbf{x}}$ denote the velocity, and consider an inertial

frame $\widetilde{K}$ moving with small velocity $\boldsymbol{\epsilon}$ relative to an inertial frame K. Then $\widetilde{\mathbf{v}} = \mathbf{v} + \boldsymbol{\epsilon}$ and $|\widetilde{\mathbf{v}}|^2 = |\mathbf{v}|^2 + 2\mathbf{v}\cdot\boldsymbol{\epsilon} + |\boldsymbol{\epsilon}|^2$, and so

$$\mathscr{L}(|\widetilde{\mathbf{v}}|^2) = \mathscr{L}(|\mathbf{v}|^2) + 2\widetilde{\mathscr{L}}(|\mathbf{v}|^2)\mathbf{v}\cdot\boldsymbol{\epsilon} + \mathcal{O}(|\boldsymbol{\epsilon}|^2). \tag{4.6}$$

However, as both frames are inertial then the two Lagrangians should be equivalent for all $\boldsymbol{\epsilon}$. Therefore the linear term of (4.6) should be a total time derivative (cf. Corollary 4.6). As the Lagrangian can only be a function of $|\mathbf{v}|^2$, then this term could only be a total time derivative if it is linear in $\mathbf{v}$. We therefore have that $\widetilde{\mathscr{L}}(|\mathbf{v}|^2)$ is independent of $\mathbf{v}$, and hence $\mathscr{L}$ is proportional to $|\mathbf{v}|^2$. This allows us to write

$$\mathscr{L} = \tfrac{1}{2}m|\mathbf{v}|^2, \tag{4.7}$$

where m is the particle's mass. Experimentally, we would observe that a particle's acceleration is inversely proportional to its mass as in section 1.1. Note that m cannot be negative since from the action (4.1) we see that Hamilton's principle would yield maxima instead of minima. We did not use the third type of Galilean transformations, but the expression (4.7) is automatically invariant with respect to rectilinear motion $\mathbf{v}' = \mathbf{v} + \mathbf{v}_0$. Indeed, we have

$$\begin{aligned}\widetilde{\mathscr{L}}(\widetilde{\mathbf{v}}) &= \tfrac{1}{2}m|\widetilde{\mathbf{v}}|^2 = \tfrac{1}{2}m|\mathbf{v}+\mathbf{v}_0|^2 = \tfrac{1}{2}m|\mathbf{v}|^2 + m\mathbf{v}\cdot\mathbf{v}_0 + \tfrac{1}{2}m\mathbf{v}_0^2 \\ &= \mathscr{L}(\mathbf{v}) + \frac{\mathrm{d}}{\mathrm{d}t}\left(m\mathbf{x}\cdot\mathbf{v}_0 + \tfrac{1}{2}m|\mathbf{v}_0|^2 t\right),\end{aligned}$$

and so the Euler–Lagrange equations are the same by Corollary 4.6.

For a system of free noninteracting particles, the Lagrangian for each individual particle cannot be dependent on the coordinates of any other, and so $\mathscr{L}$ must be additive:

$$\mathscr{L} = \sum_{i=1}^{N} \tfrac{1}{2}m_i|\mathbf{v}_i|^2 = K,$$

which yields (4.5) when there is no potential energy. In practice, to change into another coordinate system we only need to know the line element $\mathrm{d}s$ or metric $\mathrm{d}s^2$ in order to know how to transform $|\dot{\mathbf{x}}|^2$. If we wish to express the Cartesian coordinates x_i as functions of generalized coordinates $q = (q_1, \ldots, q_n)$, then we obtain

$$K = \tfrac{1}{2}\sum_{i,j=1}^{n} a_{ij}(q)\dot{q}_i\dot{q}_j \tag{4.8}$$

for functions a_{ij} of the coordinates only. That is, the kinetic energy K in generalized coordinates is still a quadratic function of velocities, but may also depend on the other coordinates. Mathematically, a conservative Lagrangian system is determined by a Riemann manifold—where the metric determines the kinetic energy—and a potential function.

To describe a general system of particles which may interact as in (4.5), we add a function to the Lagrangian. For a conservative system, this function is the potential energy:

$$\mathscr{L}(q, \dot{q}) = K(q, \dot{q}) - V(q). \tag{4.9}$$

As we are no longer in Euclidean space, we make the additional assumption that for a conservative system the force is exact (i.e. $\mathbf{F} = -\nabla V$) and not merely closed (i.e. that work is path independent). Now the time reversibility (cf. section 2.4) is easily seen as the time-independence of the Lagrangian: time reversal $t \mapsto -t$ preserves each product $\dot{q}_i\dot{q}_j$ in the quadratic kinetic energy (4.8) and thus preserves the Lagrangian (4.9). This suggests that the total energy is conserved for Lagrangians of the form (4.9); we will revisit this in more detail in Proposition 4.11.

4.3. Nonconservative systems

Thus far we have considered Lagrangians which describe conservative systems and are of the form $\mathscr{L} = K - V$. In this section we will extend Lagrangian mechanics to include nonconservative systems. We will see that the correct choice is

$$\mathscr{L} = K + W, \tag{4.10}$$

where W is the total work

$$W = \sum_{i=1}^{n} Q_i \cdot q_i \tag{4.11}$$

and Q_i are the (**generalized**) forces of the system.

It suffices to consider the case of Euclidean space as in the beginning of the proof of Proposition 4.5, but we will continue to use the notation q for convenience. Consider a system whose motion is described by the n coordinates $q_j(t) \in \mathbb{R}^d$ from time 0 to T, and consider a fixed-endpoint variation $q_j(t)+h_j(t)$. Repeating the integration by parts procedure from the proof of Proposition 4.5, we obtain

$$\begin{aligned} \mathrm{d}\bigg(\int K\,\mathrm{d}t\bigg)\bigg|_{q(t)}(h) &= \int_0^T \sum_{j=1}^{n} \left(\frac{\partial K}{\partial q_j}h_j + \frac{\partial K}{\partial \dot{q}_j}\dot{h}_j\right)\mathrm{d}t \\ &= \left[\sum_{j=1}^{n}\frac{\partial K}{\partial \dot{q}_j}h_j\right]_0^T + \int_0^T \sum_{j=1}^{n}\left(\frac{\partial K}{\partial q_j} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial K}{\partial \dot{q}_j}\right)\cdot h_j\,\mathrm{d}t \\ &= \int_0^T \sum_{j=1}^{n}\left(\frac{\partial K}{\partial q_j} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial K}{\partial \dot{q}_j}\right)\cdot h_j\,\mathrm{d}t. \end{aligned} \tag{4.12}$$

In the last equality we noted that $h_j(0) = h_j(T) = 0$ for a fixed-endpoint variation.

From (4.11) we compute the variation of the work to be

$$\mathrm{d}\bigg(\int W\,\mathrm{d}t\bigg)\bigg|_{q(t)}(h) = \int_0^T \sum_{j=1}^{n} Q_j \cdot h_j\,\mathrm{d}t. \tag{4.13}$$

Adding this in, the principle of least action for the new Lagrangian (4.10) yields

$$0 = \mathrm{d}\bigg(\int (K+W)\,\mathrm{d}t\bigg)\bigg|_{q(t)}(h) = \int_0^T \sum_{j=1}^{n}\left(\frac{\partial K}{\partial q_j} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial K}{\partial \dot{q}_j} + Q_j\right)\cdot h_j\,\mathrm{d}t.$$

As this must be true for all variations h_j, then we conclude

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial K}{\partial \dot{q}_j} - \frac{\partial K}{\partial q_j} = Q_j \quad \text{for } j = 1, \ldots, n. \tag{4.14}$$

These are **Lagrange's equations for nonconservative forces**. In other words, the motion of a nonconservative system is given by Lagrange's equations (4.4) for the Lagrangian (4.10).

We never needed to assume that the generalized forces are not conservative, and so (4.14) must reduce to the familiar formulation of Lagrange's equations when the forces are conservative. In the case $Q = -\nabla V(q)$, we can use the same integration by parts procedure in reverse to obtain

$$\begin{aligned}
&\mathrm{d}\left(\int W\,\mathrm{d}t\right)\Big|_{q(t)}(h) = \int_0^T \sum_{j=1}^n Q_j \cdot h_j\,\mathrm{d}t = -\int_0^T \sum_{j=1}^n \left[\frac{\partial V}{\partial q_j} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial V}{\partial \dot{q}_j}\right] \cdot h_j\,\mathrm{d}t \\
&= \left[\sum_{j=1}^n \frac{\partial V}{\partial \dot{q}_j} \cdot h_j\right]_0^T - \int_0^T \sum_{j=1}^n \left(\frac{\partial V}{\partial q_j} \cdot h_j + \frac{\partial V}{\partial \dot{q}_j} \cdot \dot{h}_j\right)\mathrm{d}t \\
&= -\int_0^T \sum_{j=1}^n \left(\frac{\partial V}{\partial q_j} \cdot h_j + \frac{\partial V}{\partial \dot{q}_j} \cdot \dot{h}_j\right)\mathrm{d}t = -\mathrm{d}\left(\int V\,\mathrm{d}t\right)\Big|_{q(t)}(h).
\end{aligned}$$

Therefore, the new Lagrangian (4.10) generates the same motion as the conservative Lagrangian $\mathscr{L} = K - V$.

Even when the forces are nonconservative, all we needed in the previous paragraph was the ability to write the jth component of the generalized force as

$$Q_j = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial V}{\partial \dot{q}_j} - \frac{\partial V}{\partial q_j}. \tag{4.15}$$

In this case, we recover the familiar form of Lagrange's equations (4.4) with no RHS, but now with a velocity-dependent potential $V(t, q, \dot{q})$.

The quantity $V = K - \mathscr{L}$ is called the **potential energy** even for nonconservative systems, and is generally time-dependent. A common example is a system A with coordinates q_A that is not closed, but it moves in an external field due to a system B with coordinates $q_B(t)$ independent of q_A such that the entire system $A + B$ is closed. This system has a Lagrangian of the form

$$\mathscr{L} = K_A(q_A, \dot{q}_A) - V(q_A, q_B(t)). \tag{4.16}$$

We may ignore K_B since it depends only on time and is thus a complete time derivative. Equation (4.16) is a Lagrangian of the usual type, but with V being possibly time-dependent. If system A is a single particle, then the Euler–Lagrange equations yield

$$m\ddot{q} = -\frac{\partial V}{\partial q}(t, q) = F(t, q). \tag{4.17}$$

For example, if $F \equiv F(t)$ is uniform (i.e. independent of position) then $V = \mathbf{F} \cdot \mathbf{x}$ in Euclidean space.

4.4. Equivalence to Newton's equations

Now we will see how to obtain the Euler–Lagrange equations (4.4) from Newtonian mechanics, which will show that Hamilton's principle of least action is equivalent to Newton's principle of determinacy.

A mechanical system with a configuration manifold M can always be—and in experiment is automatically—embedded in some Euclidean space $\mathbb{R}^N$. Within M, the motion of the system is dictated by some known force $\mathbf{F}$. The effect of constraining the motion to the manifold M can be thought of as a force $\mathbf{N}$ orthogonal to M, called the **constraint force**. Newton's equations for this system is

$$m_i\ddot{\mathbf{x}}_i = \mathbf{F}_i + \mathbf{N}_i.$$

Rearranging, we see that $m_i\ddot{\mathbf{x}}_i - \mathbf{F}_i = \mathbf{N}_i$ is orthogonal to M, and so

$$(m_i\ddot{\mathbf{x}}_i - \mathbf{F}_i) \cdot \boldsymbol{\xi}_i = 0$$

for all vectors $\boldsymbol{\xi} = (\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_N)$ tangent to M. This is Newton's equation in the tangent plane to the surface M. Summing over all particles, we get the **d'Alembert–Lagrange principle**:

$$\sum_{i=1}^{N} (m_i\ddot{\mathbf{x}}_i - \mathbf{F}_i) \cdot \boldsymbol{\xi}_i = 0 \tag{4.18}$$

for all vectors $\boldsymbol{\xi} \in \mathbb{R}^N$ tangent to M. In section 5.1 we will see that this principle more generally dictates the motion of a system with constraints. Note that for a free system $M = \mathbb{R}^n$ we may take any vector $\boldsymbol{\xi} \in \mathbb{R}^n$, and so we recover Newton's equations.

Let $q = (q_1, \dots, q_n)$ be local coordinates on M. Then by the chain rule we have

$$\dot{x}_i = \sum_{j=1}^{n} \frac{\partial x_i}{\partial q_j}\dot{q}_j,$$

and so we may write the kinetic energy

$$K(q, \dot{q}) = \sum_{i=1}^{N} \tfrac{1}{2} m_i |\dot{x}_i|^2 = \sum_{i,j=1}^{n} a_{ij}(q)\dot{q}_i\dot{q}_j$$

as a positive definite quadratic form on M.

Expressing the force in terms of the coordinates q_j, the covectors Q_j defined by the one-form equation

$$\sum_{i=1}^{N} F_i \,\mathrm{d}x_i = \sum_{j=1}^{n} Q_j \,\mathrm{d}q_j,$$

or equivalently

$$Q_j = \sum_{i=1}^{N} F_i \frac{\partial x_i}{\partial q_j}, \tag{4.19}$$

are called the **generalized forces**. They dictate the evolution of the kinetic energy via the following expression.

Proposition 4.9. *The Newtonian motion $q(t)$ of the system satisfies*

$$\frac{d}{dt}\frac{\partial K}{\partial \dot{q}} - \frac{\partial K}{\partial q} = Q. \tag{4.20}$$

Proof. We repeat the argument from section 4.3. The calculation (4.12) of the variation of the kinetic energy contribution still holds, since we did not use any equations of motion. Taking a dot product with an arbitrary tangent vector $\boldsymbol{\xi}$ to M, we can replace the coordinates $x \in \mathbb{R}^N$ with $q \in M$. Similarly, the calculation (4.13) still holds on M by the definition (4.19) and the d'Alembert–Lagrange principle (4.18)—that is, Newton's equations hold on the manifold M in terms of the generalized forces. Adding these together, we obtain (4.20) as desired. □

For a conservative system we have that the one-form $Q\,\mathrm{d}q$ is exact and may be written as $-\mathrm{d}V$ for a potential energy $V(q)$. For such a system we have the Lagrangian $\mathscr{L} = K - V$, and hence (4.20) implies that

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}} - \frac{\partial \mathscr{L}}{\partial q} = 0.$$

In section 4.1, we saw that this implies $q(t)$ is a critical point for the action functional. As $q(t)$ was an arbitrary motion of the system, we conclude that the principle of least action must hold.

4.5. Momentum and conservation

In this section we will investigate two special mathematical cases when we can replace a second order Euler–Lagrange equation by a first order equation, which correspond to two physically important conservation laws.

For a Lagrangian system, the **momentum** (sometimes called **generalized momentum** in physics) of a particle is defined to be

$$p_i = \frac{\partial \mathscr{L}}{\partial \dot{q}_i}. \tag{4.21}$$

If $q_i = x_i$ is a Cartesian coordinate, the kinetic energy part of the Lagrangian has a term $\frac{1}{2}m_i\dot{x}_i^2$ and so $p_i = m_i x_i$ is the linear momentum along the x_i-axis. If $q_i = \phi_i$ is the azimuthal angular coordinate in $\mathbb{R}^3$, then the kinetic energy about the z-axis is $\frac{1}{2}m_i r_i^2 \dot{\phi}_i^2$ and so $p_i = m_i r_i^2 \dot{\phi}_i$ is the angular momentum about the z-axis.

We can similarly define the (**generalized**) **force** as

$$F_i = \frac{\partial \mathscr{L}}{\partial q_i}.$$

This way, Lagrange's equations (4.4) imply

$$F_i = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}_i} = \frac{\mathrm{d}p_i}{\mathrm{d}t},$$

and so Newton's equation is still satisfied for these new quantities. This definition agrees with the one-form definition (4.19) for Q_i, and so both forces F_i and momenta p_i should be interpreted as covectors. This fact is built into the kinetic energy

$$K_i = \tfrac{1}{2}\mathbf{v}_i \cdot \mathbf{p}_i = \tfrac{1}{2}\langle \mathbf{v}_i, \mathbf{p}_i \rangle$$

on Euclidean space, since $\mathbf{v}_i = \dot{\mathbf{x}}_i$ is a tangent vector.

These definitions immediately illuminate a special case when we can replace a second order Euler–Lagrange equation by a first order equation:

Proposition 4.10 (Conservation of momentum)**.** *If a Lagrangian is independent of the variable q_i, then the corresponding momentum is conserved:*

$$\frac{\partial \mathscr{L}}{\partial \dot{q}_i} = \textit{constant}.$$

Proof. The Euler–Lagrange equations (4.4) yield

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}_i} = \frac{\partial \mathscr{L}}{\partial q_i} = 0. \qquad \square$$

Any such coordinate q_i is called **cyclic**, and so Proposition 4.10 says that if a coordinate is cyclic then the corresponding momentum is conserved. This fact includes the conservation laws we saw in Propositions 1.13 and 1.16. One of the strengths of Lagrangian mechanics is that if we can find a cyclic coordinate then there is one less equation of motion to solve. For example, in section 3.1 we picked the z-axis to align with the initial angular momentum, which eliminated the equations for the z-coordinate of the position and momentum. Cyclic coordinates can also be observed geometrically: Proposition 4.10 requires that the trajectories $q(t)$ in configuration space M lie in the level sets of p_i, and so the system has a translation symmetry in the q_i direction.

We can extend this heuristic to include the time coordinate: when the cyclic coordinate is time, then the conserved quantity is the total energy. We define the **total energy** of a system as

$$E = \sum_{i=1}^{n} \dot{q}_i p_i - \mathscr{L}. \tag{4.22}$$

This includes our previous definition, since for a conservative system on Euclidean space we have

$$\begin{aligned} E &= \sum_{i=1}^{n} v_i \frac{\partial}{\partial v_i}\left[\sum_{j=1}^{n} \tfrac{1}{2} m_j v_j^2 - V\right] - \left[\sum_{j=1}^{n} \tfrac{1}{2} m_i v_i^2 - V\right] \\ &= \sum_{i=1}^{n} m_i v_i^2 - \sum_{i=1}^{n} \tfrac{1}{2} m_i v_i^2 + V = K + V. \end{aligned}$$

Proposition 4.11 (Conservation of energy)**.** *The solution $q(t)$ to the Euler–Lagrange equations* (4.3) *satisfies*

$$E(q) = \dot{q} \cdot \frac{\partial \mathscr{L}}{\partial \dot{q}}(t, q, \dot{q}) - \mathscr{L}(t, q, \dot{q}) = \int_0^t \frac{\partial \mathscr{L}}{\partial t}(q(s), \dot{q}(s), s)\,\mathrm{d}s + \textit{constant}.$$

In particular, if the Lagrangian $\mathscr{L}$ is independent of t, then the total energy $E(q)$ is constant.

In the context of variational calculus this is sometimes called the **second Euler–Lagrange equation**, which replaces the second order equation (4.3) with a first order equation.

Proof. Using the chain rule and the Euler–Lagrange equation (4.3), we have

$$\begin{aligned}\frac{\mathrm{d}\mathscr{L}}{\mathrm{d}t} &= \frac{\partial \mathscr{L}}{\partial t} + \frac{\partial \mathscr{L}}{\partial q_i} \cdot \dot{q}_i + \frac{\partial \mathscr{L}}{\partial \dot{q}_i} \cdot \ddot{q}_i \\ &= \frac{\partial \mathscr{L}}{\partial t} + \left(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}_i}\right) \cdot \dot{q}_i + \frac{\partial \mathscr{L}}{\partial \dot{q}_i} \cdot \ddot{q}_i = \frac{\partial \mathscr{L}}{\partial t} + \frac{\mathrm{d}}{\mathrm{d}t}\left(\dot{q}_i \cdot \frac{\partial \mathscr{L}}{\partial \dot{q}_i}\right).\end{aligned}$$

Integrating in time yields the desired result. □

4.6. Noether's theorem

The conservation of momentum (Proposition 4.10) says that a system that is continuously symmetric along the coordinate q_i possesses the corresponding conserved quantity p_i. This turns out to be a general phenomenon: every one-parameter group of symmetries which preserves a Lagrangian system has a corresponding conserved quantity.

Consider a Lagrangian system consisting of a smooth n-dimensional manifold M with a time-independent Lagrangian $\mathscr{L}(t, q, v) : TM \to \mathbb{R}$. We say that a diffeomorphism $h : M \to M$ is a **symmetry** of the system if

$$\mathscr{L}(h_*(q, v)) = \mathscr{L}(q, v) \quad \text{for all } (q, v) \in TM. \tag{4.23}$$

Here, $h_*(q, v) = \mathrm{d}h(q, v)$ is the **pushforward** or **differential** of the point $q \in M$ and tangent vector $v \in T_qM$, and is equal to the point $h(q) \in M$ with the tangent vector $\mathrm{d}h|_q(v) \in T_{h(q)}M$.

Proposition 4.12 (Noether's theorem)**.** *If the Lagrangian system $(M, \mathscr{L})$ is time-independent and has a differentiable one-parameter group of diffeomorphisms $h^s : M \to M$ for $s \in \mathbb{R}$, then there is a conserved quantity (or "integral") $I : TM \to \mathbb{R}$. In local coordinates,*

$$I(q, v) = \frac{\partial \mathscr{L}}{\partial \dot{q}}(q, v) \cdot \frac{\mathrm{d}}{\mathrm{d}s} h^s(q)\bigg|_{s=0}. \tag{4.24}$$

The quantity I is independent of the choice of local coordinates q. Indeed, I measures the rate of change of $\mathscr{L}(q,v)$ as v is varied in T_qM in the direction of the tangent vector $\frac{\mathrm{d}}{\mathrm{d}s}h^s(q)|_{s=0}$, which is why the formula (4.24) looks like the chain rule for $\frac{\mathrm{d}}{\mathrm{d}s}\mathscr{L}((h^s)_*(q,v))|_{s=0}$. This does not intrinsically involve a choice of coordinates.

Proof. As in the set up for the proof of Proposition 4.5, we may fix a coordinate patch on M and take the variation to be supported within the image in order to reduce the statement to Euclidean space $\mathbb{R}^n$. Let $q(t):\mathbb{R}\to\mathbb{R}^n$ denote a solution to Lagrange's equations. As h^s is a symmetry for each s then $h^s\circ q$ will also be a solution, because $(h^s\circ q)(t)=(h^s)_*(q(t))$ is the pushforward of the point $q(t)$ and $\frac{\mathrm{d}}{\mathrm{d}t}(h^s\circ q)(t)=\mathrm{d}(h^s)\,|_{q(t)}(\dot q(t))=(h^s)_*(\dot q(t))$ is the pushforward of the tangent vector $\dot q(t)$, and so by (4.23) the Lagrangian evaluated at $(h^s\circ q)(t)$ is the same as the Lagrangian evaluated at $q(t)$.

Consider the map $\Phi:\mathbb{R}_s\times\mathbb{R}_t\to\mathbb{R}^n$ given by $\Phi(s,t)=(h^s\circ q)(t)$. As all of the symmetries h^s preserve the Lagrangian $\mathscr{L}$, then

$$0=\frac{\mathrm{d}}{\mathrm{d}s}\mathscr{L}(\Phi,\dot\Phi)=\frac{\partial\mathscr{L}}{\partial q}\cdot\frac{\partial\Phi}{\partial s}+\frac{\partial\mathscr{L}}{\partial\dot q}\cdot\frac{\partial\dot\Phi}{\partial s}, \tag{4.25}$$

where everything on the RHS is evaluated at $(\Phi(s,t),\dot\Phi(s,t))\in T\mathbb{R}^n$. As we just noted, for fixed s the map $\Phi(s,\cdot):\mathbb{R}\to\mathbb{R}^n$ satisfies the Euler–Lagrange equation

$$\frac{\partial}{\partial t}\left[\frac{\partial\mathscr{L}}{\partial\dot q}\big(\Phi(s,t),\dot\Phi(s,t)\big)\right]=\frac{\partial\mathscr{L}}{\partial q}\big(\Phi(s,t),\dot\Phi(s,t)\big).$$

Inserting this into the RHS of (4.25), we obtain

$$\begin{aligned}0&=\frac{\partial}{\partial t}\left[\frac{\partial\mathscr{L}}{\partial\dot q}\big(\Phi,\dot\Phi\big)\right]\cdot\frac{\partial\Phi}{\partial s}\big(\Phi,\dot\Phi\big)+\frac{\partial\mathscr{L}}{\partial\dot q}\big(\Phi,\dot\Phi\big)\cdot\frac{\partial\dot\Phi}{\partial s}\big(\Phi,\dot\Phi\big)\\&=\frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{\partial\mathscr{L}}{\partial\dot q}\cdot\frac{\partial\Phi}{\partial s}\right]\big(\Phi,\dot\Phi\big)=\frac{\mathrm{d}I}{\mathrm{d}t}\big(\Phi,\dot\Phi\big)\end{aligned}$$

by the chain rule. □

Example 4.13 (Translational symmetry)**.** Consider the conservative N-particle Lagrangian

$$\mathscr{L}(\mathbf{x},\mathbf{v})=\sum_{i=1}^N\tfrac12 m_i|\mathbf{v}_i|^2-V(\mathbf{x}), \tag{4.26}$$

where $\mathbf{x}=(\mathbf{x}_1,\dots,\mathbf{x}_N)$, $\mathbf{x}_i\in\mathbb{R}^d$ and similarly for $\mathbf{v}$. If the potential energy is invariant under translations along the first coordinate axis $\mathbf{e}_1\in\mathbb{R}^n$, then the system is symmetric with respect to the N translations

$$h_j^s:(\mathbb{R}^d)^N\to(\mathbb{R}^d)^N,\qquad h_j^s(\mathbf{x}_1,\dots,\mathbf{x}_N)=(\mathbf{x}_1,\dots,\mathbf{x}_j+s\mathbf{e}_1,\dots,\mathbf{x}_N)$$

for $j=1,\dots,N$. Noether's theorem yields N conserved quantities

$$I_j(\mathbf{x},\mathbf{v})=\frac{\partial\mathscr{L}}{\partial\dot{\mathbf{x}}}\cdot(0,\dots,0,\mathbf{e}_1,0,\dots,0)=m_jv_{j1},$$

which we recognize as the first component of the jth particle's momentum $\mathbf{p}_j = m_j\mathbf{v}_j$ (cf. Corollary 1.14).

Example 4.14 (Rotational symmetry)**.** Now suppose $d = 3$, and that the conservative N-particle Lagrangian (4.26) is invariant under rotations about the first coordinate axis $\mathbf{e}_1 \in \mathbb{R}^3$. Then the system is symmetric with respect to the N rotations

$$h_j^s(\mathbf{x}_1, \ldots, \mathbf{x}_N) = (\mathbf{x}_1, \ldots, \cos(s)\mathbf{x}_j + \sin(s)\mathbf{e}_1 \times \mathbf{x}_j + (1 - \cos s)x_{j1}\mathbf{e}_1, \ldots, \mathbf{x}_N)$$

for $j = 1, \ldots, N$. Noether's theorem returns the N conserved quantities

$$I_j(\mathbf{x}, \mathbf{v}) = \frac{\partial \mathscr{L}}{\partial \dot{\mathbf{x}}} \cdot (0, \ldots, 0, \mathbf{e}_1 \times \mathbf{x}_j, 0, \ldots, 0) = \mathbf{p}_j \cdot (\mathbf{e}_1 \times \mathbf{x}_j) = (\mathbf{x}_j \times \mathbf{p}_j) \cdot \mathbf{e}_1,$$

which we recognize as the first component of the jth particle's angular momentum $\mathbf{L}_j = \mathbf{x}_j \times \mathbf{p}_j$ (cf. Corollary 1.17).

4.7. Exercises

4.1 (Functional derivative is well-defined)**.** Show that if Φ is a differentiable functional, then its differential is linear and is independent of the choice in variation of γ.

4.2. Repeat the proof of Proposition 4.5 to prove the following stronger statement on Euclidean space: If $\mathscr{L} \in C^1(\mathbb{R}^n \times \mathbb{R}^n \times [0, T]; \mathbb{R})$ and $q \in C^1([0, T]; \mathbb{R}^n)$ is a (fixed-endpoint) critical point for the action functional defined in (4.1), then $\frac{\partial \mathscr{L}}{\partial \dot{q}}(t, q, \dot{q})$ is a C^1 function on $[0, T]$ and q solves the Euler–Lagrange equations (4.3).

4.3 (Geodesics on the sphere [Tro96, Ch. 1])**.** In Example 4.7 we saw that the geodesics—paths of shortest length between two given points—in $\mathbb{R}^n$ are straight lines. We will repeat this procedure for the sphere S^2.

(a) Using coordinates (ϕ, θ), we can parameterize a path $\mathbf{x}(t)$ in $S^2 \subset \mathbb{R}^3$ as

$$\mathbf{x}(t) = (\cos\phi(t)\sin\theta(t), \sin\phi(t)\sin\theta(t), \cos\theta(t)), \quad t \in [0, 1].$$

Find the formula for the arc length functional $\Phi(\mathbf{x}(t))$.

(b) After rotating the sphere we may assume that $\theta(0) = 0$, $\theta(1) = \theta_1$, and $\phi(1) = 0$. Find a simple lower bound for $\Phi[\mathbf{x}(t)]$ using the $\dot{\phi}$ term. By considering when equality occurs, conclude that the geodesic connecting the north pole $\mathbf{x}(0)$ to the point $\mathbf{x}(1)$ is the shorter arc of the great circle (an equator, or circle of maximum circumference on the sphere) connecting the two points. This is another example where we can directly confirm that the critical path for the functional is a minimum.

4.4 (Brachistochrone [Tro96, Ch. 6])**.** The brachistochrone between two points in the plane is the curve which a frictionless bead would traverse the quickest subject to a downward gravitational acceleration. Johann Bernoulli in 1696 challenged mathematicians to find the shape of the brachistochrone, and it was his brother Jakob Bernoulli who provided a solution which was later refined into the calculus of variations.

(a) After translating, we may assume that the initial point is the origin $(0, 0)$ and the second point is given by some (x_1, y_1) with $x_1 > 0$ and $y_1 < 0$. Explain why it is reasonable to assume that the brachistochrone is the graph of a function $y(x)$, $x \in [0, x_1]$ as opposed to a general parametric curve. Show that the time is takes the bead to traverse this curve is

$$\Phi[y(x)] = \int_0^{x_1} \frac{\sqrt{1 + y'(x)^2}}{v(x)} \, \mathrm{d}x$$

where $v(x)$ is the bead's speed.

(b) With constant downward acceleration g, show that $v(x) = \sqrt{2gy(x)}$.

(c) Using conservation of the energy (4.22), find the first order differential equation

$$\sqrt{\frac{y}{c^2 - y}} y' = 1.$$

(d) Introducing a new dependent variable $\theta(x)$ so that

$$y = c^2 \sin^2 \tfrac{\theta}{2} = \tfrac{1}{2} c^2 (1 - \cos\theta), \qquad 0 \le \theta < 2\pi,$$

show that

$$\tfrac{1}{2} c^2 (1 - \cos\theta)\theta' = 1.$$

(e) By integrating the two equations of the previous part, obtain the parametric equations

$$x(\theta) = c^2(\theta - \sin\theta) + c_1, \qquad y(\theta) = c^2(1 - \cos\theta).$$

In order for $x(0) = 0 = y(0)$, we must have $c_1 = 0$. That is, the brachistochrone is a cycloid; these equations describe the path traced by a fixed point on a circle of radius c^2 as it rolls along the x-axis in the lower half-plane.

4.5 (Lagrangian PDE I [Eva10, Ch. 8])**.** In this exercise we will prove the existence of a solution to the elliptic PDE

$$-\nabla \cdot (A(x)\nabla u(x)) = 0 \quad \text{for } x \in \Omega, \qquad u(x) = 0 \quad \text{for } x \in \partial\Omega,$$

on an open set $\Omega \subset \mathbb{R}^n$. Here, $A(x) = (a_{ij}(x))$ is a symmetric $n \times n$ matrix with $a_{ij} \in H^2(\Omega)$ (the Sobolev space), and we also assume that A is uniformly elliptic:

$$\lambda I \le A(x) \le \Lambda I \text{ for } x \in \Omega$$

(in the sense of positive definite matrices).

(a) For $u \in H_0^1(\Omega)$ (the closure of $C_c^\infty(\Omega)$ in $H^1(\Omega)$), show that the energy functional

$$E(u) = \tfrac{1}{2} \int_\Omega \nabla u(x) \cdot A(x) \nabla u(x) \, \mathrm{d}x$$

is finite. Show that for $\phi \in C_c^\infty(\Omega)$ the first variation at u is

$$\lim_{\epsilon \to 0} \frac{E(u + \epsilon\phi) - E(u)}{\epsilon} = \int_\Omega \nabla\phi \cdot A \nabla u.$$

Consequently, if u is a minimum of E, then the above expression vanishes for all $\phi \in C_c^\infty(\Omega)$; such a function $u \in H_0^1(\Omega)$ is called a weak solution of the PDE and boundary condition, since one formal integration by parts would produce the PDE—but we do not assume u is twice differentiable.

(b) Let u_j be a sequence in $H_0^1(\Omega)$ such that

$$\lim_{j \to \infty} E(u_j) = \inf_{H_0^1(\Omega)} E.$$

Using Poincaré's inequality, show that $E(u)$ is bounded below and hence our sequence is bounded. Conclude that there exists a weakly convergent subsequence $u_{j_k} \rightharpoonup u$ in $H^1(\Omega)$ using the Riesz representation theorem.

(c) Show that E is weakly lower semicontinuous:

$$E(u) \le \liminf_{k \to \infty} E(u_{j_k}).$$

Conclude that $u \in H_0^1(\Omega)$ is a minimum for E, and hence is a weak solution to the PDE by part (a).

4.6 (Two pendulums connected by a spring)**.** Consider two pendulums of unit length and unit mass in a constant gravitational field g. Suppose they are connected by a massless spring with spring constant k whose resting length is the same as their distance of separation.

(a) Let θ_1 and θ_2 be the angles the pendulums make with the downward verticals. Find the Lagrangian for the system for small angles, so that $\sin\theta \approx \theta$.

(b) Define new variables

$$q_1 = \frac{\theta_1 + \theta_2}{\sqrt{2}}, \quad q_2 = \frac{\theta_1 - \theta_2}{\sqrt{2}},$$

and show that Lagrangian separates into two harmonic oscillators:

$$\mathscr{L} = \tfrac{1}{2}(\dot{q}_1^2 + \dot{q}_2^2) + \tfrac{1}{2}(\omega_1^2 q_1^2 + \omega_2^2 q_2^2).$$

Find ω_1 and ω_2. When $q_2 = 0$, we have $\theta_1 = \theta_2$ and so both pendulums swing in phase with each other with frequency ω_1. When $q_1 = 0$, we have $\theta_2 = -\theta_1$ and so the pendulums swing in exact opposite phase with frequency ω_2.

(c) For $k \ll 1$ we will see that an exchange of energy occurs. Suppose that at time $t = 0$ we have $\theta_1 = 0 = \theta_2$, $\dot\theta_2 = 0$, and $\dot\theta_1 = v_0$. Using part (b), show that the motion is given by

$$\theta_1(t) = \tfrac{v_0}{2}\left(\sin t + \tfrac{1}{\omega}\sin\omega t\right), \quad \theta_2(t) = \tfrac{v_0}{2}\left(\sin t - \tfrac{1}{\omega}\sin\omega t\right)$$

with $\omega = \omega_2$. For $k \ll 1$ we have $1/\omega \approx 1$, and so

$$\theta_1(t) \approx v_0 \cos\epsilon t \sin\widetilde{\omega} t, \quad \theta_2(t) \approx -v_0 \cos\widetilde{\omega} t \sin\epsilon t$$

for some ϵ and $\widetilde{\omega}$. Show that to leading order as $k \to 0$ we have

$$\epsilon \approx \tfrac{k}{2}, \quad \widetilde{\omega} \approx 1,$$

and so after a time $T = \pi/2\epsilon \approx \pi/k$ the pendulums have switched roles and now essentially only the second pendulum is oscillating.

4.7 (Charged particle in an electromagnetic field)**.** A charged particle moving in an electromagnetic field is an example of a nonconservative Lagrangian system. A particle with charge q moving through the vector fields E, D, B, H on $\mathbb{R}^3$ with the scalar charge density ρ and vector current density j obeys Maxwell's equations (in Gaussian units):

$$\nabla \times E + \frac{1}{c}\frac{\partial B}{\partial t} = 0, \qquad \nabla \cdot D = 4\pi\rho,$$
$$\nabla \times H - \frac{1}{c}\frac{\partial D}{\partial t} = \frac{4\pi}{c} j, \qquad \nabla \cdot B = 0.$$

The force on the charge is given by the Lorentz law

$$F = q\left[E + \tfrac{1}{c}(v \times B)\right].$$

(a) The fourth Maxwell equation requires that B is divergence-free, and so we introduce a vector-valued potential A for B so that $B = \nabla \times A$. Using the first equation, introduce a scalar potential ϕ so that the electric field becomes

$$E = -\nabla\phi - \frac{1}{c}\frac{\partial A}{\partial t}$$

and the Lorentz force is

$$F = q\left[-\nabla\phi - \frac{1}{c}\frac{\partial A}{\partial t} + \frac{1}{c}(v \times (\nabla \times A))\right].$$

(b) The Lorentz force is nonconservative, but if we can put it in the form (4.15) then we will have a Lagrangian for this system. The first term $q\phi$ is already of the desired form. Show that the x-component of the rightmost term $v \times (\nabla \times A)$ may be rewritten as

$$(v \times (\nabla \times A))_x = \frac{\partial}{\partial x}(v \cdot A) - \frac{\mathrm{d}A_x}{\mathrm{d}t} + \frac{\partial A_x}{\partial t}.$$

By symmetry, we get the same relation for the other components with x replaced by the respective variable.

(c) Show that the x-component of the Lorentz force can be written as

$$F_x = -\frac{\partial V}{\partial x} + \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial V}{\partial v_x}$$

for the potential energy

$$V = q\phi - \tfrac{q}{c} v \cdot A.$$

Symmetrically, the y- and z-components of the Lorentz force are also of this form if we replace x with the respective coordinates. Consequently, the Lagrangian for this system is

$$\mathscr{L} = K - V = \tfrac{1}{2} m v^2 - q\phi + \tfrac{q}{c} v \cdot A$$

where m is the particle's mass.

4.8 (Noether's theorem with time dependence)**.** Consider a Lagrangian system $\mathscr{L} : \mathbb{R} \times TM \to \mathbb{R}$ with time dependence.

(a) Prove an extension of Noether's theorem for this system by applying Proposition 4.12 to the extended configuration space $M_1 = M \times \mathbb{R}$ with Lagrangian

$$\mathscr{L}_1\left(q, t, \frac{\mathrm{d}q}{\mathrm{d}\tau}, \frac{\mathrm{d}t}{\mathrm{d}\tau}\right) = \mathscr{L}\left(q, \frac{\mathrm{d}q/\mathrm{d}\tau}{\mathrm{d}t/\mathrm{d}\tau}, t\right)\frac{\mathrm{d}t}{\mathrm{d}\tau}$$

and the new time variable τ, to obtain a conserved quantity $I(t, q, \dot{q})$ on M.

(b) Apply this to a time-independent Lagrangian $\mathscr{L}(t, q, v) \equiv \mathscr{L}(q, v)$ to conclude that the total energy is conserved.

4.9 (Lagrangian PDE II)**.** In this exercise, we will explore the formal Lagrangian structure associated with the wave equation. The Lagrangian formulation of the wave equation (as opposed to the Hamiltonian formulation) is advantageous because it shares the Lorentz symmetries of the wave equation. For further details, see [SS98].

(a) Let

$$g = \begin{pmatrix} -1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix} = (g_{\alpha\beta})_{\alpha,\beta=0,\ldots,d}$$

denote the $(d+1) \times (d+1)$ matrix associated with the Minkowski metric $\mathrm{d}s^2 = -\mathrm{d}t^2 + \mathrm{d}x_1^2 + \cdots + \mathrm{d}x_d^2$ on $\mathbb{R}_t \times \mathbb{R}_x^d$, with coordinates $(x_0, \ldots, x_d) = (t, x_1, \ldots, x_d)$. Consider the Lagrangian

$$\mathscr{L}(u, \nabla u) := \sum_{\alpha,\beta=0}^{d} (g^{-1})_{\alpha\beta} \frac{\partial u}{\partial x_\alpha}\frac{\partial u}{\partial x_\beta} + F(u) = -\tfrac{1}{2}\left|\tfrac{\partial u}{\partial t}\right|^2 + \tfrac{1}{2}|\nabla u|^2 + F(u).$$

Show formally that a function $u : \mathbb{R} \times \mathbb{R}^d \to \mathbb{C}$ is a critical point for the action

$$S(u) := \int_{\mathbb{R}\times\mathbb{R}^d} L(u, \nabla u)\sqrt{-\det g}\,\mathrm{d}x\,\mathrm{d}t$$

if and only if u solves the (semilinear) wave equation

$$-\tfrac{\partial^2 u}{\partial t^2} + \Delta u = F'(u).$$

(b) Now we will take $F \equiv 0$ and derive the conservation laws of the linear wave equation. Consider the same Lagrangian $\mathscr{L}(u, \nabla u, g)$ and action $S(u, g)$ to be functions of the metric g. Given $\tau : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R} \times \mathbb{R}^d$ a smooth and compactly supported diffeomorphism, let g_s, $s \in \mathbb{R}$ be the pullback of the metric g by the map $\mathrm{id} + s\tau$, so that

$$(g_s)_{\alpha\beta}\big|_{s=0} = g_{\alpha\beta}, \qquad \tfrac{\mathrm{d}}{\mathrm{d}s}(g_s)_{\alpha\beta}\big|_{s=0} = \tfrac{\partial \tau_\beta}{\partial x_\alpha} + \tfrac{\partial \tau_\alpha}{\partial x_\beta} =: \pi_{\alpha\beta}.$$

Similarly, let u_s be the pullback of the metric g by the map $\mathrm{id} + s\tau$, so that $u_s|_{s=0} = u$. Using that $\frac{\mathrm{d}}{\mathrm{d}s} S(u_s, g_s)|_{s=0} = 0$ for all diffeomorphisms τ (because the Lagrangian is invariant under the change of variables $(t, x) \mapsto (t, x) + s\tau(t, x)$), show formally that if u is a critical point for $S(u, g)$ then

$$\int_{\mathbb{R}\times\mathbb{R}^d} \sum_{\alpha,\beta=0}^{d} T^{\alpha\beta}\pi_{\alpha\beta}\sqrt{-\det g}\,\mathrm{d}x\,\mathrm{d}t = 0,$$

where

$$T^{\alpha\beta} := \tfrac{\partial \mathscr{L}}{\partial (g^{-1})_{\alpha\beta}} - \tfrac{1}{2} g_{\alpha\beta}\mathscr{L}$$

is the **stress-energy tensor**. Conclude that $T^{\alpha\beta}$ is divergence-free:

$$\sum_{\alpha=0}^{d} \tfrac{\partial T^{\alpha\beta}}{\partial x_\alpha} = 0 \quad \text{for } \beta = 0, \dots, d.$$

These yield the microscopic conservation laws

$$\tfrac{\partial T^{00}}{\partial t} + \sum_{k=1}^{d} \tfrac{\partial T^{0k}}{\partial x_k} = 0, \qquad \tfrac{\partial T^{0j}}{\partial t} + \sum_{k=1}^{d} \tfrac{\partial T^{jk}}{\partial x_k} = 0 \quad \text{for } j = 1, \dots, d.$$

(c) Integrate in space to formally show that the total energy

$$E(u) := \int_{\mathbb{R}^d} T^{00}(t, x)\,\mathrm{d}x = \int_{\mathbb{R}^d} \left(\tfrac{1}{4}\left|\tfrac{\partial u}{\partial t}\right|^2 + \tfrac{1}{4}|\nabla u|^2\right)\mathrm{d}x$$

and the components of the momentum

$$p_j(u) := \int_{\mathbb{R}^d} T^{0j}(t, x)\,\mathrm{d}x = -\tfrac{1}{2}\int_{\mathbb{R}^d} \mathrm{Re}\left(\tfrac{\partial u}{\partial t}\overline{\tfrac{\partial u}{\partial x_j}}\right)\mathrm{d}x \quad \text{for } j = 1, \dots, d$$

are conserved. These are the corresponding macroscopic conservation laws.

CHAPTER 5

CONSTRAINTS

In this chapter we explore some physical and mathematical formulations of constraints. Note that this does not include methods of solving the equations of constrained motion; cf. [AKN06, Sec. 1.6]. The treatment of holonomic constraints is based on [AKN06, Ch. 1], the treatment of nonholonomic constraints is based on [Gol51, Ch. 1–2], and section 5.5 is based on [MZ05].

5.1. D'Alembert–Lagrange principle

A **holonomic constraint** on a Lagrangian system $(M, \mathscr{L})$ is the requirement that the system's motion is confined to a submanifold S of the phase space TM that locally can be expressed by

$$f_1(t, q, \dot{q}) = \cdots = f_k(t, q, \dot{q}) = 0. \tag{5.1}$$

A constraint that is not holonomic is called a **nonholonomic constraint**.

Example 5.1. Rigid-body motion in Euclidean space $\mathbb{R}^d$ requires that the distance between any two particles $\mathbf{x}_i \in \mathbb{R}^d$ is fixed. This is a holonomic constraint because it can be expressed as

$$|\mathbf{x}_i - \mathbf{x}_j|^2 - c_{ij}^2 = 0, \tag{5.2}$$

where c_{ij} are the inter-particle distances.

Conversely, the motion of particles $\mathbf{x}_i \in \mathbb{R}^d$ confined to a rigid spherical container of radius R centered at the origin is a nonholonomic constraint, because it is given by

$$|\mathbf{x}_j|^2 - R^2 \leq 0.$$

Both of these examples happen to be time-independent, but this need not be the case.

In this section, we will assume that we have a holonomic constraint. A vector $\xi \in T_qM$ is tangent to the submanifold S provided that

$$\frac{\partial f_1}{\partial \dot{q}}(t, q, \dot{q}) \cdot \xi = \cdots = \frac{\partial f_k}{\partial \dot{q}}(t, q, \dot{q}) \cdot \xi = 0. \tag{5.3}$$

Such a vector ξ is called a **virtual velocity** of the constrained motion at the state $(q, \dot{q}) \in TM$ and time t. We can ensure that the motion $q(t)$ is constrained to S by insisting that

$$\left(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}} - \frac{\partial \mathscr{L}}{\partial q}\right) \cdot \xi = 0 \tag{5.4}$$

for all virtual velocities ξ at the state $(q(t), \dot{q}(t))$.

Definition 5.2 (d'Alembert–Lagrange principle)**.** A motion of the Lagrangian system $(M, \mathscr{L})$ subject to the holonomic constraints (5.1) is a smooth trajectory solving (5.4) for all virtual velocities ξ.

By the definition (5.3) of the virtual velocities, this requires that the LHS of the Euler–Lagrange equations be within the span of the derivatives $\frac{\partial f_i}{\partial \dot{q}}$. In other words, there exist constants $\mu_1, \ldots, \mu_k$ so that

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}} - \frac{\partial \mathscr{L}}{\partial q} = \sum_{i=1}^{k} \mu_i \frac{\partial f_i}{\partial \dot{q}} \tag{5.5}$$

These are called **Lagrange's equations with multipliers**. Mathematically, we recognize the constants μ_i as Lagrange multipliers: in order for the action functional to obtain a minimum on the submanifold S, the gradient of the action (the LHS of (5.5)) must be orthogonal to the submanifold S. Physically, if we imagine that the particle system is confined to the submanifold S via fictitious **constraint forces** given by the RHS of (5.5) (cf. section 4.4), then (5.4) states that the constraint forces must be orthogonal to the motion and hence do no work.

We can also observe the constraint effect in terms of the principle of least action and the admissible path variations. Given a path $\gamma \in \Omega$, let Γ be the subspace of the tangent space $T_\gamma \Omega$ consisting of vectors W where W_t is a virtual velocity for each t. For holonomic constraints, the following proposition states that the constrained Lagrangian system on M is given by a the principle of least action on S, and hence the system's degrees of freedom are effectively reduced.

Proposition 5.3 (Hölder's principle)**.** *A path $\gamma \in \Omega$ is a motion of the Lagrangian system with the holonomic constraints S if and only if the functional derivative $\mathrm{d}S|_\gamma$ of the action vanishes on the subspace Γ.*

Proof. By Proposition 4.5, the first derivative of the action S at the path $q(t)$ in the direction of the fixed-endpoint variation $H_s(t)$ is

$$\mathrm{d}S|_\gamma\left(\frac{\partial H_s}{\partial s}\right) = \int_0^T \left(\frac{\partial \mathscr{L}}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}}\right) \cdot \frac{\partial H_s}{\partial s}\,\mathrm{d}t.$$

Restricting $\mathrm{d}S|_\gamma$ to the subspace Γ is equivalent to requiring that $\frac{\partial H_s}{\partial s}$ is a virtual velocity. As every virtual velocity can be attained by some variation $\frac{\partial H_s}{\partial s}$, we see from the above variation that $\mathrm{d}S|_\gamma$ vanishes on Γ if and only if the d'Alembert–Lagrange principle (5.4) is satisfied. □

Example 5.4. We can think of the pendulum of Example 4.8 as a particle of mass m in a vertical plane $(x, y) \in \mathbb{R}^2$ subject to a downward gravitational force with potential $V(x, y) = mgy$ and to the holonomic constraints

$$x^2 + y^2 - \ell^2 = 0, \qquad 2x\dot{x} + 2y\dot{y} = 0,$$

where ℓ is the length of the pendulum arm. Note that the second condition is a time derivative of the first equation, but is necessary to specify the two-dimensional submanifold S in the four-dimensional tangent space $T\mathbb{R}^2 = \mathbb{R}^2 \times \mathbb{R}^2$. If we let θ denote the angle from the downward vertical and r the distance from the pivot, then the Lagrangian becomes

$$\mathscr{L} = \tfrac{1}{2}m(r^2\dot{\theta}^2 + \dot{r}^2) + mgr\cos\theta,$$

and the holonomic conditions are

$$f_1(r, \theta, \dot{r}, \dot{\theta}) = r^2 - \ell^2 = 0, \qquad f_2(r, \theta, \dot{r}, \dot{\theta}) = \dot{r} = 0.$$

The first constraint does not place any restrictions on the virtual velocities $\xi = (\xi_r, \xi_\theta)$ since $\frac{\partial f_1}{\partial(\dot{r},\dot{\theta})} = 0$, but the second condition yields

$$0 = \frac{\partial f_2}{\partial(\dot{r}, \dot{\theta})} \cdot \xi = \xi_r.$$

The d'Alembert–Lagrange principle (5.4) then yields the condition

$$(m\ddot{r} - mr\dot{\theta}^2 - mg\cos\theta)\xi_r + (mr^2\ddot{\theta} + 2mr\dot{r}\dot{\theta} + mgr\sin\theta)\xi_\theta = 0.$$

As $\xi_r = 0$ and ξ_θ is arbitrary, we conclude that the second parenthetical term above vanishes. After using the constraints f_1 and f_2, we obtain the familiar equation of motion

$$\ddot{\theta} = -\tfrac{g}{\ell}\sin\theta.$$

The holonomic constraints have effectively discarded the r equation and reduced the degrees of freedom from two to one.

5.2. Gauss' principle of least constraint

Unlike the principle of least action, the d'Alembert–Lagrange principle is not an optimization problem due to the presence of the virtual velocities. Gauss sought to recast the constrained system as an optimization problem, and he discovered that the actual constrained motion is the feasible constrained motion which deviates the least from the unconstrained motion.

The state of the system at time 0 is determined by the position $q_0 = q(0)$ and velocity $v_0 = \dot{q}(0)$ at a fixed time, and then the acceleration $a(0) = \ddot{q}(0)$ is determined by the laws of motion and constraints. Consequently, we will consider q_0 and v_0 as fixed while we vary a_0. For a fixed state $(q_0, v_0) \in TM$ and time 0, we will refer to all paths $q(t)$ allowed by the constraints with $q(0) = q_0$

and $\dot{q}(0) = v_0$ as the **conceivable motions**; these lie in the constraint submanifold S but do not necessarily satisfy the equations of motion. A **released motion** satisfies the unconstrained Euler–Lagrange equations (4.4) (and does not lie in S), and an **actual motion** is a conceivable motion satisfying the d'Alembert–Lagrange principle (5.4) (and hence lies in S).

By considering only variations supported in a fixed coordinate patch, we may reduce to a neighborhood about the point q_0 and work in Euclidean coordinates with the vector notation $q(t) = \mathbf{x}(t)$. We will write an actual motion of the system $\mathbf{x}_a(t) = \mathbf{x}_r(t) + \delta\mathbf{x}(t)$ as a deviation from the released motion $\mathbf{x}_r(t)$, and we assume that the initial positions $\mathbf{x}_a(0) = \mathbf{x}_r(0) = \mathbf{x}_0$ and velocities $\dot{\mathbf{x}}_a(0) = \dot{\mathbf{x}}_r(0) = \mathbf{v}_0$ are fixed. Taylor expanding we have

$$\begin{aligned}\mathbf{x}_r(t) &= \mathbf{x}_0 + t\mathbf{v}_0 + \tfrac{1}{2}t^2\ddot{\mathbf{x}}_r(0) + \mathcal{O}(t^3),\\ \mathbf{x}_a(t) &= \mathbf{x}_0 + t\mathbf{v}_0 + \tfrac{1}{2}t^2\ddot{\mathbf{x}}_a(0) + \mathcal{O}(t^3).\end{aligned}$$

Therefore we have

$$\delta\mathbf{x}(t) = \tfrac{1}{2}t^2\delta\ddot{\mathbf{x}}(0) + \mathcal{O}(t^3). \tag{5.6}$$

So far, we have not yet used the constraints.

In our local coordinates the d'Alembert–Lagrange principle requires

$$\left(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathscr{L}}{\partial\dot{\mathbf{x}}} - \frac{\partial\mathscr{L}}{\partial\mathbf{x}}\right)\cdot\boldsymbol{\xi} = 0 \tag{5.7}$$

for all virtual velocities $\boldsymbol{\xi}$. For conservative systems, $\frac{\partial\mathscr{L}}{\partial\mathbf{x}}$ is the system's force $-\nabla V$ and $\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathscr{L}}{\partial\dot{\mathbf{x}}}$ is the total force $m\ddot{\mathbf{x}}$ (i.e. the system's force plus the fictitious constraint forces). So in this special case, we see that $\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathscr{L}}{\partial\dot{\mathbf{x}}} - \frac{\partial\mathscr{L}}{\partial\mathbf{x}}$ is the force $m\,\delta\ddot{\mathbf{x}}$ due to the constraints. In the general case, we evaluate $\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathscr{L}}{\partial\dot{\mathbf{x}}} - \frac{\partial\mathscr{L}}{\partial\mathbf{x}}$ at $\mathbf{x}_a(t) = \mathbf{x}_r(t) + \delta\mathbf{x}(t)$ and Taylor expand about $\mathbf{x}_r(t)$:

$$\begin{aligned}\left(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathscr{L}}{\partial\dot{\mathbf{x}}} - \frac{\partial\mathscr{L}}{\partial\mathbf{x}}\right)\bigg|_{\mathbf{x}=\mathbf{x}_a} &= \left(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathscr{L}}{\partial\dot{\mathbf{x}}} - \frac{\partial\mathscr{L}}{\partial\mathbf{x}}\right)\bigg|_{\mathbf{x}=\mathbf{x}_r}\\ &+ \left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial^2\mathscr{L}}{\partial\dot{\mathbf{x}}^2}\delta\dot{\mathbf{x}} + \frac{\partial^2\mathscr{L}}{\partial\dot{\mathbf{x}}\partial\mathbf{x}}\delta\mathbf{x}\right) - \frac{\partial^2\mathscr{L}}{\partial\mathbf{x}^2}\delta\mathbf{x} - \frac{\partial^2\mathscr{L}}{\partial\dot{\mathbf{x}}\partial\mathbf{x}}\delta\dot{\mathbf{x}}\right]_{\mathbf{x}=\mathbf{x}_r} + \mathcal{O}(|\delta\mathbf{x}|^2).\end{aligned}$$

The first term on the RHS vanishes since the released motion $\mathbf{x}_r$ solves Lagrange's equations. For the second term, we use (5.6) and take the limit $t \to 0$ to obtain

$$\left(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathscr{L}}{\partial\dot{\mathbf{x}}} - \frac{\partial\mathscr{L}}{\partial\mathbf{x}}\right)\bigg|_{\substack{\mathbf{x}=\mathbf{x}_a\\ t=0}} = \frac{\partial^2\mathscr{L}}{\partial\dot{\mathbf{x}}^2}\bigg|_{\substack{\mathbf{x}=\mathbf{x}_r\\ t=0}}\delta\ddot{\mathbf{x}}(0).$$

Therefore, we see that (5.7) requires

$$\frac{\partial^2\mathscr{L}}{\partial\dot{q}^2}\bigg|_{\substack{q=q_r\\ t=0}}(\ddot{q}_a(0) - \ddot{q}_r(0)) \tag{5.8}$$

to be orthogonal to the constraint submanifold S. On the other hand, (5.8) is the gradient of the functional

$$Z(q(t)) = \tfrac{1}{2}(\ddot{q} - \ddot{q}_r) \cdot A(\ddot{q} - \ddot{q}_r)\big|_{t=0} \tag{5.9}$$

for the Hessian matrix $A = \frac{\partial^2 \mathscr{L}}{\partial \dot{q}^2}$ of the kinetic energy quadratic form at $\mathbf{x} = \mathbf{x}_r$ and $t = 0$. For conservative systems, A is a positive definite matrix containing the particle masses. The quantity (5.9) is called Gauss' **compulsion**, and it measures how much the motion $q(t)$ deviates from the released motion.

As the gradient (5.8) of the compulsion functional (5.9) evaluated at the actual motion q_a is orthogonal to the submanifold S, we conclude that the actual motion q_a is a critical point for the compulsion functional. Moreover, all that we used to prove this was that the constants μ_i in (5.5) are Lagrange multipliers. In fact, the converse of this statement is also true. Let $f(q)$ be a smooth functional on M with a critical point q_a when restricted to the submanifold S. This happens if and only if $D(f \circ \phi)|_{q_a} = 0$ for all coordinates ϕ from Euclidean space to a neighborhood of q_a in S. Writing $D(f \circ \phi) = \nabla f \cdot D\phi$ and noting that the columns of the matrix $D\phi$ span the tangent space $T_q S \subset T_q M$, we conclude that q_a is a critical point on S if and only if the gradient $\nabla f(q_a) \in T_q M$ is orthogonal $T_q S$.

Altogether, we have proven the following:

Theorem 5.5 (Gauss' principle)**.** *Among the conceivable motions, the actual motion $q(t)$ is a critical point for the compulsion* (5.9) *with respect to the released motion. In particular, if A is positive definite then the actual motion is the global minimum for the compulsion with respect to the released motion.*

See Exercise 5.1 for an example of Gauss' principle.

Gauss' principle is analogous to the method of least squares in regression analysis (which was also discovered by Gauss). In the method of least squares, there is an unknown data correlation function determined by n parameters and a large number $N > n$ of observations. The observations deviate slightly from the desired function's exact values due to observation error, and hence the overdetermined system for the correlation function is inconsistent. The remedy is to construct the square sum error between the correlation function and the data, and then find the desired function as an error minimizer in the n parameters. Here, the compulsion is determined by the $2n$ initial conditions $(q_0, v_0) \in TM$ where $n = \dim M$ is the number of degrees of freedom, and the system is overdetermined due to the extra constraint conditions. Here, the actual motion $q(t)$ plays the role of the function we seek determined by the smaller number of conditions $\dim TS < 2n$, the released motion is the measured data which overdetermines the correlation function with error, and the compulsion is the square sum error. Moreover, the matrix A of masses can statistically be interpreted as weights in the method of least squares, which are modified based on the assumed reliability of the data accuracy.

5.3. Integrability

Some authors also require that holonomic constraints are integrable (in the sense of Frobenius). In this section, we will explore what this additional assumption yields.

In this section, we will assume that the motion is constrained within a k-dimensional **distribution** $\Delta \subset TM$: for any $q_0 \in M$, Δ_{q_0} is a k-dimensional subspace of $T_{q_0}M$ and there exist smooth vector fields $X_1, \dots, X_k$ defined on a neighborhood of q_0 such that Δ_q is given by the span of $X_1(q), \dots, X_k(q)$ on that neighborhood. For holonomic constraints, Δ is the space of virtual velocities. We will also assume that Δ is **integrable**: there exists an embedding $i : N \to M$ such that $\mathrm{d}i(T_qN) = \Delta_q$ for all $q \in N$; in other words, Δ is given by the tangent bundle of a submanifold.

Frobenius' theorem provides us with a practical condition to determine if the distribution Δ is integrable:

Theorem 5.6 (Frobenius' theorem)**.** *The distribution Δ is integrable if and only if Δ is **involutive**—that is, for any vector fields $X, Y \in \Delta$, the Lie bracket $[X, Y]$ is also in Δ.*

This abstract result expresses a basic idea when applied to differential equations: a first-order system of equations can be solved locally if and only if they are consistent. For example, consider a function $u = (u_1, \dots, u_m)$ of the variables $q = (q_1, \dots, q_k)$ which solves the system of equations

$$\frac{\partial u}{\partial q_1}(q) = F_1(q, u), \quad \dots, \quad \frac{\partial u}{\partial q_k}(q) = F_k(q, u).$$

Of course, if there exists a solution u, then the right-hand sides $F_1, \dots, F_k$ must be consistent:

$$\begin{aligned} \frac{\partial}{\partial q_j} F_i(q, u(q)) &= \frac{\partial^2 u}{\partial q_i \partial q_j}(q) = \frac{\partial}{\partial q_i} F_j(q, u(q)) \\ \implies \quad \frac{\partial F_i}{\partial q_j} + \frac{\partial F_i}{\partial u} \cdot F_j &= \frac{\partial F_j}{\partial q_i} + \frac{\partial F_j}{\partial u} \cdot F_i \end{aligned}$$

for all i and j. This is the involutive condition of Forbenius' theorem. Moreover, the theorem also provides the converse: if the right-hand sides $F_1, \dots, F_k$ are consistent, then there exists a local solution. For a proof of Frobenius' theorem, see [Lee13, Th. 19.12].

If the holonomic constraints are integrable, then the motion $q(t)$ must lie in a submanifold of M, not merely a submanifold of TM. Now that we know that the holonomic constraints have a corresponding smooth integrable submanifold $N \subset M$ of dimension $d-k$, we can show that the d'Alembert–Lagrange condition is equivalent to the principle of least action holding on N:

Proposition 5.7. *Suppose the Lagrangian system $(M, \mathscr{L})$ has integrable holonomic constraints. Then a constrained path is a motion of the system if and only if the path is a motion for the system $(N, \mathscr{L}|_N)$.*

Proof. From Hölder's principle (Proposition 5.3) we know that the d'Alembert–Lagrange condition is equivalent to insisting that the action variation $\mathrm{d}S|_\gamma$ vanishes on a subspace Γ of conceivable variations. Here, Γ is a subspace of the tangent space $T_{q(t)}\Omega_M$ to the paths Ω_M on M. On the other hand, the motion of the Lagrangian system on N is given by taking the action S on the paths Ω_N on N, and then insisting that its variation vanishes on the tangent space $T_{q(t)}\Omega_N$. The key observation is that the tangent space $T_{q(t)}\Omega_N$ is equal to the subspace Γ, and so the two conditions are identical. □

In particular, the motion for integrable holonomic constraints is determined by the restriction of the Lagrangian to the constraint submanifold N. In this way, a system with holonomic constraints is like a new mechanical system with fewer degrees of freedom; this is a characteristic feature of holonomic constraints, which we do not expect for nonholomic constraints.

5.4. Integral constraints

In this section, we will assume we have a Lagrangian system $(M, \mathscr{L})$ subject to the constraint

$$\int_0^T G(q(t))\,\mathrm{d}t = 0, \tag{5.10}$$

for some smooth $G : M \to \mathbb{R}$ that is not a constant function.

Proposition 5.8. *If $q(t)$ is a critical point for a functional $S(q(t))$ of the form* (4.1) *subject to the constraint* (5.10) *and $G(q(t))$ is nonconstant, then there exists a Lagrange multiplier $\lambda \in \mathbb{R}$ so that $q(t)$ solves*

$$\frac{d}{dt}\frac{\partial \mathscr{L}}{\partial \dot{q}} - \frac{\partial \mathscr{L}}{\partial q} = \lambda \frac{\partial G}{\partial q}. \tag{5.11}$$

Proof. As in the set up for the proof of Proposition 4.5, we may fix a coordinate patch on M and take the variation to be supported within the image in order to reduce the statement to Euclidean space $\mathbb{R}^n$. Let $q(t) : \mathbb{R} \to \mathbb{R}^n$ be a critical point, and let $g = \frac{\partial G}{\partial q}$ denote the gradient of G. By premise, we know that $g(q) \not\equiv 0$. In particular, there exists a smooth function $v(t) : \mathbb{R} \to \mathbb{R}^n$ so that

$$\int_0^T g(q(t)) \cdot v(t)\,\mathrm{d}t \neq 0. \tag{5.12}$$

Let $h(t)$ be a fixed-endpoint variation. To obtain a differential equation for $q(t)$ we would like to perturb $q(t)$ by the variation $h(t)$. However, the perturbed path $q(t) + h(t)$ will not satisfy the constraint for arbitrary $h(t)$, and so we will need to modify our perturbation. Let

$$J(\sigma, \tau) := \int_0^T G\big(q(t) + \sigma h(t) + \tau v(t)\big)\,\mathrm{d}t.$$

We claim there is a smooth function $\tau(\sigma)$ defined on a neighborhood of zero such that $\tau(0) = 0$ and

$$J(\sigma, \tau(\sigma)) \equiv 0 \quad \text{for all } \sigma. \tag{5.13}$$

This follows from the implicit function theorem, since we know that $J(0,0) = 0$ and

$$\frac{\partial J}{\partial \tau}(0,0) = \int_0^T g(q(t)) \cdot v(t)\,\mathrm{d}t$$

is nonzero by (5.12).

The perturbation $q + \sigma h + \tau(\sigma)v$ now satisfies the constraint for all σ sufficiently small. As $q(t)$ is a critical point of the constrained action functional, then we must have

$$0 = \frac{\mathrm{d}}{\mathrm{d}\sigma} \int_0^T \mathscr{L}\big(q + \sigma h + \tau(\sigma)v, \dot{q} + \sigma\dot{h} + \tau(\sigma)\dot{v}, t\big)\,\mathrm{d}t.$$

Using the derivative of the action functional (4.2), we have

$$0 = \int_0^T \left[\frac{\partial \mathscr{L}}{\partial q}(q) - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}}(q)\right] \cdot (h + \tau'(0)w)\,\mathrm{d}t. \tag{5.14}$$

On the other hand, differentiating (5.13) with respect to σ we obtain

$$\begin{aligned} 0 = \frac{\mathrm{d}}{\mathrm{d}\sigma}\big[J(\sigma, \tau(\sigma))\big]_{\sigma=0} &= \frac{\partial J}{\partial \sigma}(0,0) + \frac{\partial J}{\partial \tau}(0,0)\,\tau'(0) \\ &= \int_0^T g(q(t)) \cdot h(t)\,\mathrm{d}t + \tau'(0)\int_0^T g(q(t)) \cdot v(t)\,\mathrm{d}t, \end{aligned}$$

and so

$$\tau'(0) = -\frac{\int_0^T g(q(t)) \cdot h(t)\,\mathrm{d}t}{\int_0^T g(q(t)) \cdot v(t)\,\mathrm{d}t}.$$

Inserting this into the derivative (5.14) we arrive at

$$0 = \int_0^T \left[\frac{\partial \mathscr{L}}{\partial q}(q) - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}}(q) + \lambda g(q)\right] \cdot h\,\mathrm{d}t,$$

where

$$\lambda = -\frac{\int_0^T \left[\frac{\partial \mathscr{L}}{\partial q}(q) - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}}(q)\right] \cdot w(t)\,\mathrm{d}t}{\int_0^T g(q(t)) \cdot v(t)\,\mathrm{d}t}$$

is independent of h. As $h(t)$ was an arbitrary fixed-endpoint variation, we conclude that (5.11) holds. □

5.5. Existence of closed orbits

In this section we will assume that we have a time-independent Lagrangian $\mathscr{L}(q, \dot{q})$. By Proposition 4.11, we know that the total energy

$$E = \dot{q} \cdot \frac{\partial \mathscr{L}}{\partial \dot{q}} - \mathscr{L} \tag{5.15}$$

is conserved. For a conservative Lagrangian of the form

$$\mathscr{L}(q, \dot{q}) = \sum_{i=1}^{n} \tfrac{1}{2} m_i \dot{q}_i^2 - V(q), \tag{5.16}$$

this yields the usual expression

$$E(q, \dot{q}) = \sum_{i=1}^{n} \tfrac{1}{2} m_i \dot{q}_i^2 + V(q).$$

For such a system, we seek closed orbits (i.e. periodic solutions) to Lagrange's equations. We will explore some well-known results in this field obtained by variational methods, and then settle our attention on the proof of one specific result (Theorem 5.12 below). For each result, closed orbits are produced by proving the existence of an optimizer for a certain variational problem. To this end, it is more convenient to work with the energy (5.15) instead of the Lagrangian (5.16) since it is convex when V is. Consequently, these results are more naturally phrased in terms of Hamiltonian mechanics, even though they fall under the topic of optimization and constraints.

For one-dimensional systems, we know from section 2.5 that there are many periodic trajectories. However, the following example illustrates that closed orbits can be quite exceptional for $n \geq 2$ degrees of freedom.

Example 5.9. Consider two particles of mass $m = 1$ moving according to the two-dimensional harmonic oscillator potential

$$V(x_1, x_2) = \tfrac{1}{2}(k_1 x_1^2 + k_2 x_2^2),$$

where $k_1, k_2 > 0$ are constants. Then Newton's system of equations decouple, and x_1 and x_2 are independent harmonic oscillators with constants k_1 and k_2 respectively. We found the equations of motion in Example 2.2, and $x_1(t)$ and $x_2(t)$ are each periodic with periods $2\pi/\sqrt{k_1}$ and $2\pi/\sqrt{k_2}$ respectively. Therefore, when $k_1 = k_2$ then all trajectories for $x = (x_1, x_2)$ are periodic, and when $\sqrt{k_1/k_2}$ is merely rational we still have infinitely many periodic trajectories. However, when $\sqrt{k_1/k_2}$ is irrational, only trajectories with $x_1 \equiv p_1 \equiv 0$ or $x_2 \equiv p_2 \equiv 0$ are periodic, and every other trajectory is aperiodic.

Nevertheless, under mild assumptions, there is still must be some closed orbits. A classical result in this vein is the following theorem of Lyapunov:

Theorem 5.10. *Suppose $E : \mathbb{R}^{2n} \to \mathbb{R}$ has a minimum at $x = 0$ with $E''(0)$ positive definite, and suppose that the eigenvalues of $E''(0)$ satisfy $\lambda_k/\lambda_\ell \notin \mathbb{Z}$ for $k \neq \ell$. Then Lagrange's equations* (4.4) *have n distinct periodic orbits on the surface $E(x) = \epsilon$ for all $\epsilon > 0$ sufficiently small.*

The proof follows Poincaré's perturbation method and is elementary, but is still rather clever; cf. [MZ05, §2.2]. Note that we cannot guarantee more than n closed orbits, as Example 5.9 illustrates. On the other hand, whether the assumption that $\lambda_k/\lambda_\ell \notin \mathbb{Z}$ is necessary remains an open question.

Another notion of a flow-invariant family of trajectories is that of geodesics in differential geometry. In that setting, we have the following result:

Theorem 5.11. *A smooth compact surface in $\mathbb{R}^d$ whose interior is convex admits d closed nonconstant and non-self-intersecting geodesics.*

The existence of at least one closed geodesic is a famous result of Birkhoff, and the improvement to d closed geodesics was later made by Lusternik and Schnirelmann. (Note that d is the right number of geodesics, as can be seen by an ellipsoid in $\mathbb{R}^3$.) Birkoff's idea was to rephrase the question as a minimax problem (cf. [Str08, Th. 4.4]): given an ellipsoid-like object in $\mathbb{R}^3$, we want to pass it through a rubber band while stretching the band the least. Specifically, if we take $\theta \in \mathbb{R}/2\pi\mathbb{Z}$ and $\phi \in [0, \pi]$ to be coordinates on the sphere S^2, our rubber band is given by a ϕ-dependent closed loop $\ell_\phi(\theta)$ with ℓ_0 being a constant function at the north pole and ℓ_π being the south pole. We then take the maximum stretch of ℓ_ϕ in θ, and then minimize in ϕ.

For the remainder of this section, we will focus on the following result of Weinstein [Wei78] and Rabinowitz [Rab78] and its proof:

Theorem 5.12. *Suppose we have a conservative Lagrangian of the form* (5.16). *If $\{x \in \mathbb{R}^{2n} : E(x) \leq E_0\}$ is convex, then Lagrange's equations* (4.4) *have a closed orbit on the surface $E(x) = E_0$.*

To prove Theorem 5.12, we will extract the trajectory $x(t) = (q(t), \dot{q}(t))$ as a minimizer of a functional. Our first idea for a variational principle might be the principle of least action, which can rewrite using (5.15) as follows: if $x : \mathbb{R}/T\mathbb{Z} \to \mathbb{R}^{2n}$ is a critical point of

$$\int_0^T \left[E(x(t)) - \tfrac{1}{2}\dot{x}(t) \cdot Jx(t)\right] \mathrm{d}t, \quad \text{where} \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix},$$

then $x(t)$ solves

$$\dot{x} = J\nabla E(x) \tag{5.17}$$

(and this is a first-order rewriting of Lagrange's equations (4.4) for our Lagrangian (5.16)). However, it is not clear how to guarantee the existence of a minimizer, because the integrand of the functional above is the difference of convex functions and hence is not convex.

On the other hand, the total energy E by itself is convex. Consequently, our next guess might be to seek critical points $x : \mathbb{R}/T\mathbb{Z} \to \mathbb{R}^{2n}$ for

$$\int_0^T E(x(t))\,\mathrm{d}t, \quad \text{subject to the constraint} \quad \int_0^T \tfrac{1}{2}\dot{x}\cdot Jx\,\mathrm{d}t = 1.$$

Then, arguing as in Proposition 5.8, a critical point $x(t)$ must satisfy

$$\nabla E(x) = -\lambda J\dot{x} \quad \Longrightarrow \quad \lambda\dot{x} = J\nabla E(x)$$

for a Lagrange multiplier $\lambda \in \mathbb{R}$. If $\lambda = 0$, then $\nabla E(x(t)) \equiv 0$ and so $x(t)$ is a curve of fixed points. If $\lambda \neq 0$, then the rescaling $y(t) := x(t/\lambda)$ is a periodic solution to (5.17) with period $|\lambda|T$. Although this functional is convex, it turns out that it is difficult to obtain enough control over $E(x)$ to prove Theorem 5.12.

Our proof of Theorem 5.12 will be based on the following idea (which is due to Clarke [Cla79]): it is easier to control the Legendre transform $F = E^*$, the object that is dual to the convex function E, rather than E itself. We will study this transformation more thoroughly in section 7.2 when it arises naturally in the study of Hamiltonian mechanics, and so we defer the proofs of some basic facts (cf. Theorem 7.5) which we will borrow.

Proposition 5.13 (Clarke's dual action principle)**.** *Suppose that E and F are strictly convex smooth functions on $\mathbb{R}^{2n}$ such that $F = E^*$ (cf. the premise of Theorem 7.5). If $z : \mathbb{R}/T\mathbb{Z} \to \mathbb{R}^{2n}$ is a critical point for*

$$\int_0^T F(\dot{z})\,dt \quad \textit{subject to} \quad \int_0^T \tfrac{1}{2}\dot{z}\cdot Jz\,dt = 1 \quad \textit{and} \quad \int_0^T z\,dt = 0,$$

then there exist $\lambda > 0$ and $\beta \in \mathbb{R}^{2n}$ so that

$$y = \lambda Jz + \beta \quad \textit{solves} \quad \dot{y} = \lambda J\nabla E(y).$$

That is, y is a time-scaled periodic solution to (5.17)*.*

Proof. Let $\phi : \mathbb{R}/T\mathbb{Z} \to \mathbb{R}^{2n}$ be a smooth function with $\int_0^T \phi\,\mathrm{d}t = 0$. Given a critical point $z(t)$, there must exist a Lagrange multiplier $\lambda \in \mathbb{R}$ so that

$$0 = \int \left[\nabla F(\dot{z})\cdot\dot{\phi} + \lambda\phi\cdot J\dot{z}\right]\mathrm{d}t = \int \left[\nabla F(\dot{z})\cdot\dot{\phi} - \lambda\dot{\phi}\cdot Jz\right]\mathrm{d}t.$$

In the last equality we integrated by parts, and the boundary terms canceled by periodicity. As $\dot{\phi}$ can be an arbitrary smooth periodic function, then we conclude that we must have

$$\nabla F(\dot{z}) - \lambda Jz = \beta. \tag{5.18}$$

Next, we set $y = \lambda Jz + \beta$. As $F = E^*$, we have $\nabla F = (\nabla E)^{-1}$ (cf. the calculation (7.6) and (7.7) in Theorem 7.5) and hence y solves

$$\dot{y}(t) = \lambda J\nabla E(y(t)).$$

It only remains to show that $\lambda > 0$. By the equation (5.18) for z, we have

$$\begin{aligned} 0 &= \int_0^T \dot{z} \cdot \left[\nabla F(\dot{z}) - \lambda J z - \beta\right] \mathrm{d}t \\ &= \int_0^T \dot{z} \cdot F(\dot{z})\, \mathrm{d}t - \lambda \int_0^T \dot{z} \cdot Jz\, \mathrm{d}t - \int_0^T \dot{z} \cdot \beta\, \mathrm{d}t. \end{aligned}$$

The third integral on the RHS vanishes by periodicity, and the second integral is equal to 2 by the constraint. As F is strictly convex, we must have $\xi \cdot \nabla F(\xi) > 0$ for all $\xi \neq 0$. Altogether, we conclude that $\lambda \geq 0$. If $\lambda = 0$ then we have $\dot{z} \equiv 0$, but this contradicts the constraints. □

In the proof we used that $\dot{z} \not\equiv 0$, which implies that z cannot be identically constant and so y cannot vanish identically. It then follows that y can never vanish, because $x = 0$ is the unique point where $\nabla E = 0$ and so $y(t) = 0$ implies $y(t) \equiv 0$.

In applying Proposition 5.13 to prove Theorem 5.12, there is a problem: the solution produced by Proposition 5.13 is on some nonzero energy surface, but not necessarily the one we started with. To solve this issue, we will modify E so that it is positive homogeneous of degree 2:

$$\widetilde{E}(\lambda x) = \lambda^2 \widetilde{E}(x) \quad \text{for all } x \in \mathbb{R}^{2n},\ \lambda > 0$$

without changing the level surface $E = E_0$. As E is strictly convex with minimum zero, then for each unit vector $\nu \in \mathbb{R}^{2n}$, $|\nu| = 1$ there is a unique $r(\nu)$ so that

$$E(r(\nu)\nu) = c.$$

We then define

$$\widetilde{E}(x) = c|x|^2 r(\nu)^{-2}$$

for $x \neq 0$ and $\widetilde{E}(0) = 0$, so that $E = E_0$ and $\widetilde{E} = E_0$ correspond to the same level surface. Lastly, we check that if we can find a closed orbit for $\widetilde{E}$, then we also have a closed orbit for E. As $E = E_0$ and $\widetilde{E} = E_0$ are the same surface and ∇E and $\nabla \widetilde{E}$ are perpendicular to this surface, then there must exist a proportionality constant $s(x)$ so that

$$\nabla \widetilde{E}(x) = s(x) \nabla E(x).$$

(We may assume that ∇E is nonvanishing on the surface $E = E_0$, since otherwise we can take $x(t)$ to be identically constant.) This means that solutions to

$$\dot{x} = J \nabla \widetilde{E}(x) \quad \text{and} \quad \dot{x} = J \nabla E(x)$$

only differ in time-parameterization. Therefore, replacing E by $\widetilde{E}$, we may assume that E is positive homogeneous of degree 2.

Now suppose that $z(t)$ is a solution in the sense of Proposition 5.13. Then $E(z(t))$ is constant, but perhaps not equal to E_0. As E is positive homogeneous

of degree 2 and $z(t)$ is nonvanishing, then $E(z(t)) > 0$ and so we may choose $\lambda > 0$ so that $x(t) = \lambda z(t)$ satisfies $E(x(t)) \equiv E_0$. Using that E is homogeneous again, we see that

$$\dot{x} = \lambda J \nabla E(z) = J \nabla E(x)$$

as desired.

In order to extract a minimizer, we will use the following fact from functional analysis:

Lemma 5.14 (Mazur's lemma)**.** *Let X be a Banach space. If we have a weakly convergent sequence $x_n \rightharpoonup x$ in X, then there exists a sequence of finite convex combinations of the x_n that converge strongly to x.*

Proof. Let $\mathscr{C}$ denote the set of finite convex combinations of the sequence elements x_n, which is clearly convex. If the statement of the lemma were false, then by Hahn–Banach there would exist a linear functional ℓ^* so that

$$\sup\{\ell(y) : y \in \mathscr{C}\} < \ell(x).$$

This contradicts that $\ell(x_n) \to \ell(x)$, as is guaranteed by weak convergence. □

To conclude the proof of Theorem 5.12, it suffices to show:

Proposition 5.15. *The functional $z \mapsto \int_0^{2\pi} F(\dot{z})\, dt$ achieves its minimum over the set*

$$\left\{ z : \mathbb{R}/2\pi\mathbb{Z} \to \mathbb{R}^{2n} \ : \ \int |\dot{z}|^2 \, dt < \infty, \ \int z \, dt = 0, \ \tfrac{1}{2} \int \dot{z} \cdot Jz \, dt = 1 \right\}.$$

Indeed, after rescaling time, by Proposition 5.13 we obtain a nontrivial periodic solution $z(t)$ to (5.17). As we have assumed that E is homogeneous of degree 2, then a constant multiple $x(t) = \lambda z(t)$ lies on the energy surface $E = E_0$ and is a still a periodic solution. (This solution is in the space $H^1(\mathbb{R}/2\pi\mathbb{Z})$ and thus only solves the equation pointwise almost everywhere at first, but a standard bootstrap argument shows that it must in fact be infinitely smooth.)

Proof. Let z_n be an optimizing sequence. As

$$c|x|^2 \leq F(x) \leq C|x|^2$$

for some constants $c, C > 0$, we see that the functional is well-defined on its domain and that the optimizing sequence z_n is in $H^1(\mathbb{R}/2\pi\mathbb{Z})$. (Note that the domain is also nonempty, since it contains harmonic oscillators like those in Example 5.9.)

Decompose the z_n as the Fourier series

$$z_n(t) = \sum_{k \in \mathbb{Z} \smallsetminus \{0\}} \widehat{z}_n(k) e^{ikt}.$$

(Note that $\widehat{z}_n(0) = \int z \, \mathrm{d}t = 0$ by the constraints.) By Parseval we have

$$2\pi \sum_{k \neq 0} k^2 |\widehat{z}_n(k)|^2 = \int |z_n|^2 \, \mathrm{d}t \leq \tfrac{1}{c} \int F(\dot{z}_n) \, \mathrm{d}t. \tag{5.19}$$

The RHS converges as the sequence z_n is minimizing, and hence is bounded uniformly in n. Therefore, by Bolzano–Weierstrass we may pass to a subsequence along which each $\widehat{z}_n(k)$ converges to some $\widehat{z}(k)$ as $n \to \infty$. These values are indeed Fourier coefficients for some $z(t)$ by the upper bound (5.19). The function $z(t)$ is then also real-valued since $\widehat{z}(-k) = \overline{\widehat{z}(k)}$, and $z(t)$ also satisfies the constraint $\int z \, \mathrm{d}t = \widehat{z}(0) = 0$. For the second constraint, we have

$$1 = \tfrac{1}{2} \int \dot{z}_n \cdot J z_n \, \mathrm{d}t = \pi \sum_{k \neq 0} ik \widehat{z}_n(k) \cdot J \widehat{z}_n(-k).$$

We know the RHS converges by dominated convergence, since each summand converges and we have the uniform bound (5.19). (Alternatively this follows immediately from the Rellich–Kondrashov compactness theorem for the embedding $H^1(\mathbb{R}/2\pi\mathbb{Z}) \hookrightarrow H^{1/2}(\mathbb{R}/2\pi\mathbb{Z})$, but here we have a simple direct argument.)

Altogether, we now have a function $z(t)$ that satisfies the constraints. In order to conclude that z is a minimizer, it only remains to show that the functional $\int_0^{2\pi} F(\dot{z}) \, \mathrm{d}t$ is weakly lower semicontinuous: if $z_n \rightharpoonup z$ weakly in $H^1(\mathbb{R}/2\pi\mathbb{Z})$, then

$$\int F(\dot{z}) \, \mathrm{d}t \leq \liminf_{n \to \infty} \int F(\dot{z}_n) \, \mathrm{d}t.$$

(This follows immediately from Tonelli's theorem in functional analysis, but we will provide a direct proof.) As $z_n \rightharpoonup z$ weakly in $H^1(\mathbb{R}/2\pi\mathbb{Z})$, by Mazur's lemma (Lemma 5.14) and a diagonal argument there exist finite convex combinations $\sum_{m \geq n} p_{n,m} z_m$ that converge to z in $H^1(\mathbb{R}/2\pi\mathbb{Z})$. As F is convex, then we have

$$\begin{aligned} \int F(\dot{z}) \, \mathrm{d}t &= \lim_{n \to \infty} \int F\biggl(\sum_{m \geq n} p_{n,m} \dot{z}_m \biggr) \, \mathrm{d}t \\ &\leq \lim_{n \to \infty} \sum_{m \geq n} p_{n,m} \int F(\dot{z}_m) \, \mathrm{d}t \\ &\leq \limsup_{n \to \infty} \int F(\dot{z}_n) \, \mathrm{d}t. \end{aligned}$$

Therefore, after initially replacing z_n by a subsequence which converges to $\liminf \int_0^{2\pi} F(\dot{z}_n)$, then the RHS above is $\liminf \int_0^{2\pi} F(\dot{z}_n)$ as desired. □

5.6. One-form constraints

In the derivation of Lagrange's equations (Proposition 4.5), the last step relied upon the generalized coordinates q_j being independent. As discussed in section 5.3, such q_j can always be chosen for a system subject to (integrable)

holonomic constraints. This is not always true in the nonholonomic case however, and so we would like to develop a new tool for this situation.

Suppose we have m nonholonomic constraints that can be expressed as the vanishing of one-forms:

$$\sum_{k=1}^{n} a_{\ell k}(t,q)\,\mathrm{d}q_k + a_{\ell t}(t,q)\,\mathrm{d}t = 0 \quad \text{for } \ell = 1,\dots,m. \tag{5.20}$$

Note that velocity-independent holonomic constraints also fit this requirement, because if the condition (5.1) is independent of $\dot{q}$ then taking the differential of both sides yields

$$\sum_{k=1}^{n} \frac{\partial f}{\partial q_k}\,\mathrm{d}q_k + \frac{\partial f}{\partial t}\,\mathrm{d}t = 0.$$

However, the constraint (5.20) also includes some nonholonomic constraints; for example, see (5.29) of Exercise 5.4.

Consider fixed-endpoint variations $\delta q(t)$ of a path $q(t)$ between the times 0 and T as in the proof of Proposition 4.5. The constraint (5.20) is satisfied for $q(t)$, and so Taylor expansion yields

$$\sum_{k=1}^{n} a_{\ell k}(t,q)\,\delta q_k = \mathcal{O}(\delta q^2) \quad \text{for } \ell = 1,\dots,m. \tag{5.21}$$

If there were no constraints, the principle of least action would require

$$\int_0^T \sum_{k=1}^{n} \left(\frac{\partial \mathscr{L}}{\partial q_k} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}_k} \right) \delta q_k\,\mathrm{d}t = 0. \tag{5.22}$$

To make (5.21) look like this, we multiply by coefficients λ_ℓ to be chosen, sum over ℓ, and integrate from 0 to T:

$$\int_0^T \sum_{k=1}^{n} \sum_{\ell=1}^{m} \lambda_\ell a_{\ell k} \delta q_k\,\mathrm{d}t = \mathcal{O}(\delta q^2).$$

Adding this to (5.22) we obtain

$$\int_0^T \sum_{k=1}^{n} \left(\frac{\partial \mathscr{L}}{\partial q_k} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}_k} + \sum_{\ell=1}^{m} \lambda_\ell a_{\ell k} \right) \delta q_k\,\mathrm{d}t = \mathcal{O}(\delta q^2). \tag{5.23}$$

The n generalized coordinates q_k are not independent since they are related by the m constraints. However, the first $n-m$ coordinates can be chosen independently, and the remaining m coordinates are determined by the conditions (5.21). Pick the multipliers λ_ℓ such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}_k} - \frac{\partial \mathscr{L}}{\partial q_k} = \sum_{\ell=1}^{m} \lambda_\ell a_{\ell k} \quad \text{for } n-m < k \le n. \tag{5.24}$$

This causes the last m terms of the summation in the variation (5.23) to vanish, leaving us with

$$\int_0^T \sum_{k=1}^{n-m} \left(\frac{\partial \mathscr{L}}{\partial q_k} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathscr{L}}{\partial \dot{q}_k} + \sum_{\ell=1}^{m} \lambda_\ell a_{\ell k} \right) \delta q_k \, \mathrm{d}t = \mathcal{O}(\delta q^2).$$

As the first $n-m$ coordinates q_k are independent, then we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathscr{L}}{\partial \dot{q}_k} - \frac{\partial \mathscr{L}}{\partial q_k} = \sum_{\ell=1}^{m} \lambda_\ell a_{\ell k} \quad \text{for } k = 1, \ldots, n-m.$$

Including our choice (5.24) of the last m coordinates, we conclude

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathscr{L}}{\partial \dot{q}_k} - \frac{\partial \mathscr{L}}{\partial q_k} = \sum_{\ell=1}^{m} \lambda_\ell a_{\ell k} \quad \text{for all } k = 1, \ldots, n. \tag{5.25}$$

This is the extension of **Lagrange's equations for nonholonomic constraints**. Note that these are n equations in $n+m$ unknowns—the n coordinates q_k and the m multipliers λ_ℓ. To make the system not under-determined, we must also consider the m equations:

$$\sum_{k=1}^{d} a_{\ell k} \dot{q}_k + a_{\ell t} = 0 \quad \text{for } \ell = 1, \ldots, m,$$

obtained from the one-form constraints (5.20). Comparing these new equations of motion (5.25) to the generalization for nonconservative forces (4.14), we see that the quantities $\sum_\ell \lambda_\ell a_{\ell k}$ are a manifestation of the constraint forces.

5.7. Exercises

5.1. For the pendulum of Example 5.4, explicitly verify that minimizing the compulsion Z leads to the familiar equation of motion.

5.2 (Hoop rolling down an inclined plane)**.** Consider a circular disk of mass M and radius r rolling without slipping due to gravity down a stationary inclined plane of fixed inclination ϕ.

(a) In a vertical plane, the disk requires three coordinates: two Cartesian coordinates (x, y) for the center of mass and an angular coordinate to measure the disk's rotation. If we pick the origin such that the surface of the inclined plane is the line $y = r - (\tan\phi)x$, obtain a holonomic constraint of the form (5.1) for the center of mass corresponding to the disk sitting on the plane.

(b) Consequently, we now can pick two generalized coordinates to describe the disk's motion: let x denote the distance of the disk's point of contact

and the top of the inclined plane, and θ the angle through which the disk has rotated from its initial state. By considering the arc length through which the disk has rolled, show that rolling without slipping poses another holonomic constraint.

(c) In this case, it is easier to treat rolling without slipping as a nonholonomic constraint of the type in section 5.6:

$$r\,\mathrm{d}\theta - \mathrm{d}x = 0.$$

Show that the Lagrangian for this system is

$$\mathscr{L} = \tfrac{1}{2}M(\dot{x}^2 + r^2\dot{\theta}^2) + Mgx\sin\phi.$$

(d) Apply Lagrange's equations of the form (5.25) to determine the equations of motion. Here, λ is the force of friction that causes the disk to roll without slipping. Using the differential equation of constraint

$$r\dot{\theta} = \dot{x},$$

conclude that

$$\ddot{x} = \tfrac{g}{2}\sin\phi, \qquad \ddot{\theta} = \tfrac{g}{2r}\sin\phi, \qquad \lambda = \tfrac{Mg}{2}\sin\phi.$$

5.3 (Catenary [Tro96, Ch. 3])**.** The catenary is the shape taken by a cable hung by both ends subject to gravity.

(a) Consider a cable of length L hung between two equal height supports separated by a distance $H < L$. Let y denote the vertical coordinate with $y = 0$ at the point where the cable is fastened, and let $y(s)$ denote the shape of the cable where s is the arc length along the cable, so that $y(0) = 0 = y(L)$. If the weight per unit length is a constant W, explain why the cable shape $y(s)$ minimizes the mass integral

$$F[y(s)] = W\int_0^L y(s)\,\mathrm{d}s.$$

If we instead chose the horizontal coordinate x as the independent variable, it turns out that the resulting functional would not be convex.

(b) The functional with Lagrangian $(t, y, y') \mapsto Wy$ is merely convex rather than strictly convex, and consequently may not have a unique minimizer. Show that in order to span the supports, the cable must satisfy the constraint

$$\int_0^L \sqrt{1 - y'(s)^2}\,\mathrm{d}s = H.$$

(Note that $|y'(s)| = 1$ requires $x'(s) = 0$, which would produce a cusp.) The new Lagrangian

$$\mathscr{L}(t, y, y') = Wy - \lambda\sqrt{1 - y'^2}$$

is strictly convex for $\lambda > 0$.

(c) Apply the Euler–Lagrange equation and integrate once to obtain the first order differential equation

$$\frac{\lambda y'(s)}{\sqrt{1-y'^2(s)}} = s + c$$

for the catenary, where c is a constant.

(d) As we expect $y(s)$ to be unique by convexity, there is no harm in making additional assumptions. Assume that the cable shape is symmetric about the midpoint $\ell = L/2$, and conclude that $y'(\ell) = 0$ and $c = -\ell$. Solve for $y'(s)$ and integrate on $[0, s]$ to obtain

$$y(s) = \sqrt{\lambda^2 + (\ell - s)^2} - \sqrt{\lambda^2 + \ell^2} \quad \text{on } [0, \ell].$$

(e) Show that the constraint of part (b) yields

$$\int_0^\ell \frac{\lambda}{\sqrt{\lambda^2 + (\ell - s)^2}}\, \mathrm{d}s = \frac{H}{2}.$$

Make the substitution $\ell - s = \lambda \sinh\theta$, evaluate the integral, and conclude that

$$\lambda = \frac{\ell}{\sinh(H/L)}.$$

(f) Show that $x(s)$ is given by

$$x(s) = \int_0^s \sqrt{1 - y'(t)^2}\, \mathrm{d}t = \frac{H}{2} - \lambda \sinh^{-1}\left(\frac{\ell - s}{\lambda}\right).$$

Together with $y(s)$ from part (d), we have parametric equations for the catenary. Eliminate the variable s and conclude

$$y(x) = \lambda \cosh\left(\frac{x - \frac{H}{2}}{\lambda}\right) - \sqrt{\lambda^2 + \ell^2}$$

for $x \in [0, H]$. That is, the catenary is the graph of hyperbolic cosine.

(g) Obtain the same expression for $y(x)$ using Proposition 5.8.

5.4 (Solving Kepler's problem with harmonic oscillators [KS65])**.** Consider the system of section 3.3, where a particle $\mathbf{x} \in \mathbb{R}^3$ of mass m moves in a central potential

$$V(|\mathbf{x}|) = -\frac{Mm}{|\mathbf{x}|}.$$

Recall that the squaring function on $\mathbb{C} \simeq \mathbb{R}^2$ given by

$$u := u_1 + iu_2 = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \mapsto x := u^2 = \begin{pmatrix} u_1^2 - u_2^2 \\ 2u_1 u_2 \end{pmatrix} \tag{5.26}$$

is conformal (except at the origin) and maps conic sections centered at the origin to conic sections with one focus at the origin. As the orbits $\mathbf{x}(t)$ are conic sections, we might hope to apply a transformation with similar properties to our system in order to turn the elliptic orbits into simple harmonic oscillation. (As a problem-solving method this may seem rather *ad hoc*, but an analogous transformation was used to solve a long-standing open problem in physics.)

Associated to (5.26) is the the linear transformation

$$\begin{pmatrix} \mathrm{d}x_1 \\ \mathrm{d}x_2 \end{pmatrix} = 2 \begin{pmatrix} u_1 & -u_2 \\ u_2 & u_1 \end{pmatrix} \begin{pmatrix} \mathrm{d}u_1 \\ \mathrm{d}u_2 \end{pmatrix}$$

of differential forms. The matrix above has the following key properties:

- its entries are linear homogeneous functions of the u_i,
- it is like an orthogonal matrix, in the sense that the dot product of any two rows vanishes and each row has norm $u_1^2 + u_2^2 + \cdots + u_n^2$.

We would like to find such a transformation on $\mathbb{R}^n$. It turns out that algebraically such transformations can only exist for $n = 1$, 2, 4, or 8. Ultimately we want a transformation $\mathbb{R}^n \to \mathbb{R}^3$, so we take $n = 4$ and choose a matrix

$$A = \begin{pmatrix} u_1 & -u_2 & -u_3 & u_4 \\ u_2 & u_1 & -u_4 & -u_3 \\ u_3 & u_4 & u_1 & u_2 \\ u_4 & -u_3 & u_2 & -u_1 \end{pmatrix}$$

which satisfies these properties. (This matrix also can be obtained directly from quaternion multiplication.) Consequently, we set

$$\begin{pmatrix} \mathrm{d}x_1 \\ \mathrm{d}x_2 \\ \mathrm{d}x_3 \\ 0 \end{pmatrix} = 2A \begin{pmatrix} \mathrm{d}u_1 \\ \mathrm{d}u_2 \\ \mathrm{d}u_3 \\ \mathrm{d}u_4 \end{pmatrix} = 2 \begin{pmatrix} u_1\,\mathrm{d}u_1 - u_2\,\mathrm{d}u_2 - u_3\,\mathrm{d}u_3 + u_4\,\mathrm{d}u_4 \\ u_2\,\mathrm{d}u_1 + u_1\,\mathrm{d}u_2 - u_4\,\mathrm{d}u_3 - u_3\,\mathrm{d}u_4 \\ u_3\,\mathrm{d}u_1 + u_4\,\mathrm{d}u_2 + u_1\,\mathrm{d}u_3 + u_2\,\mathrm{d}u_4 \\ u_4\,\mathrm{d}u_1 - u_3\,\mathrm{d}u_2 + u_2\,\mathrm{d}u_3 - u_1\,\mathrm{d}u_4 \end{pmatrix}. \tag{5.27}$$

Sadly, only the first three of these equations are exact forms, corresponding to the quantities

$$\begin{aligned} x_1 &= u_1^2 - u_2^2 - u_3^2 + u_4^2, \\ x_2 &= 2(u_1u_2 - u_3u_4), \\ x_3 &= 2(u_1u_3 + u_2u_4) \end{aligned} \tag{5.28}$$

respectively. The fourth equation of (5.27) is the nonholonomic constraint

$$u_4\,\mathrm{d}u_1 - u_3\,\mathrm{d}u_2 + u_2\,\mathrm{d}u_3 - u_1\,\mathrm{d}u_4 = 0. \tag{5.29}$$

Equation (5.28) defines a transformation from $\mathbb{R}^4$ into $\mathbb{R}^3$, and in fact there are explicit formulas for both the one-dimensional kernel and the inverse map.

(a) Let $r = |\mathbf{x}|$ denote the distance to the origin in $\mathbb{R}^3$. Show that

$$u_1^2 + u_2^2 + u_3^2 + u_4^2 = r.$$

Using the orthogonality of A, invert the transformation (5.27) of differentials and conclude that for a fixed point $u \in \mathbb{R}^4$ our transformation conformally maps the space orthogonal to the kernel at u onto $\mathbb{R}^3$.

(b) Let $u, v \in \mathbb{R}^4$ be two orthonormal vectors which satisfy the condition

$$u_4 v_1 - u_3 v_2 + u_2 v_3 - u_1 v_4 = 0,$$

inspired by the constraint (5.29). From part (a) we know that the plane $\operatorname{span}\{u, v\}$ is mapped conformally onto a plane in $\mathbb{R}^3$. Show that when this transformation is restricted to $\operatorname{span}\{u, v\}$ onto its image, distances from the origin are squared and angles at the origin are doubled. (Hint: The calculation of the image x of a point in $\operatorname{span}\{u, v\}$ is rather lengthy. To finish, it may help to compare the formula for x to the formula for Cayley–Klein parameters (cf. [Gol51, Sec. 4.5]).)

(c) In particular, it follows that a conic section centered at the origin in the plane $\operatorname{span}\{u, v\} \subset \mathbb{R}^4$ gets mapped to another conical section in $\mathbb{R}^3$ with one focus at the origin, the latter of which describes Kepler's motion. Using part (b) and polar coordinates in the plane $\operatorname{span}\{u, v\}$, show that ellipses and hyperbolas in the plane $\operatorname{span}\{u, v\}$ centered at the origin are mapped to ellipses and hyperbolas respectively, and from the limit case conclude that a line in $\operatorname{span}\{u, v\}$ is mapped to a parabola.

(d) We want to take the motion $x(t) \in \mathbb{R}^3$ subject to the force $P = (P_1, P_2, P_3)$ and transpose it into motion $u(t)$ in $\mathbb{R}^4$ subject to the force $Q = (Q_1, Q_2, Q_3, Q_4)$ and the constraint (5.29). Use the transformation of differentials (5.27) to determine the kinetic energy K and the force Q in terms of the coordinates u and forces P, and use the formula for the force Q to show that

$$u_4 Q_1 - u_3 Q_2 + u_2 Q_3 - u_1 Q_4 = 0. \tag{5.30}$$

(e) Apply Lagrange's equations (4.14) for nonconservative forces to obtain the equations of motion for $u(t)$. These equations have Q_i on the RHS, so add them together according to the identity (5.30), simplify, and integrate once to obtain

$$r(u_4 \dot{u}_1 - u_3 \dot{u}_2 + u_2 \dot{u}_3 - u_1 \dot{u}_4) = \text{constant}. \tag{5.31}$$

The parenthetical term above is exactly the constraint (5.29) divided by $\mathrm{d}t$, and so to ensure that the constraint is upheld we pick the initial conditions for u and $\dot{u}$ so that the parenthetical term vanishes initially, and hence for all time by the conservation of (5.31). (Conversely, it can be shown that the equations of motion for $u(t)$ and the condition $u_4 \dot{u}_1 - u_3 \dot{u}_2 + u_2 \dot{u}_3 - u_1 \dot{u}_4 = 0$ yield $m\ddot{x} = P$.)

(f) The equations of motion for u have a singularity at $r = 0$. To deal with this, change variables $t \mapsto s$ where s is the regularizing time

$$s = \int_0^t \frac{\mathrm{d}t}{r}, \quad \text{so that} \quad \frac{\mathrm{d}}{\mathrm{d}t} = \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}s}.$$

Insert the Kepler forces $Q_i = -\partial V(r)/\partial u_i$ and the (signed) semi-major axis

$$a_0 = \left(\frac{2}{r} - \frac{v^2}{M}\right)^{-1}$$

to arrive at

$$\frac{\partial^2 u_i}{\partial s^2} + \frac{M}{4a_0} u_i = 0.$$

That is, the preimage of bounded orbits ($a_0 > 0$) under this transformation is simple harmonic motion in $\mathbb{R}^4$ with frequency $\omega = \sqrt{M/4a_0}$. The harmonic motion can be (rather tediously) transformed into a solution $u(t)$ by computing and substituting in the physical time $t = \int_0^s r(s)\,\mathrm{d}s$.

CHAPTER 6

HAMILTON–JACOBI EQUATION

Rather than n second-order ODEs, the Hamilton–Jacobi equation of motion is one partial differential equation in $2n + 1$ variables. The material for this chapter is based on [LL76, Ch. 7] and [Gol51, Ch. 9].

6.1. Hamilton–Jacobi equation

In this section, we will derive the Hamilton–Jacobi equation of motion. To begin, we return our attention to the action functional.

As in section 4.1, consider the variation of the action $S(q)$ at the systems motion $q(t)$ for paths with fixed endpoints. After fixing a coordinate patch, we can reduce to an open subset of Euclidean space (cf. the proof of Proposition 4.5). Write the variation of the actual motion $q(t)$ between times 0 and T as $q(t) + \delta q(t)$. Previously we assumed $\delta q(0) = \delta q(T) = 0$ and then prescribed the resulting variation δS to vanish in accordance with the principle of least action. Now we will consider how the action $S(t, q(t))$ varies as a function of the coordinates at time T by allowing $\delta q(T)$ to vary.

Repeating the calculation of the action variation from Proposition 4.5, we now have

$$\mathrm{d}S|_q(\delta q) = \left[\frac{\partial \mathscr{L}}{\partial \dot{q}} \cdot \delta q\right]_0^T + \int_0^T \left(\frac{\partial \mathscr{L}}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}}\right) \cdot \delta q \,\mathrm{d}t = \frac{\partial \mathscr{L}}{\partial \dot{q}}(t) \cdot q(t).$$

The integral vanishes as $q(t)$ satisfies Lagrange's equations of motion. On the other hand, now only one of the boundary terms vanish since $\delta q(0) = 0$. If we let $t := T$ vary now, then we conclude

$$\frac{\partial S}{\partial q_i} = \frac{\partial \mathscr{L}}{\partial \dot{q}_i} = p_i. \tag{6.1}$$

In the last equality, we used the definition (4.21) of the generalized momentum.

By definition (4.1) of the action we have

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \mathscr{L}. \tag{6.2}$$

On the other hand, the chain rule applies to $S = S(t, q(t))$ insists

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \frac{\partial S}{\partial t} + \frac{\partial S}{\partial q} \cdot \dot{q} = \frac{\partial S}{\partial t} + p \cdot \dot{q} \tag{6.3}$$

by (6.1). Setting (6.2) and (6.2) equal yields

$$\frac{\partial S}{\partial t} = \mathscr{L} - p \cdot \dot{q} = -H,$$

where H is the total energy (or Hamiltonian) (4.22). Using the derivative (6.1), we recognize this identity as a first order partial differential equation (PDE) for $S(t, q)$:

Theorem 6.1. *If $q(t)$ is a critical point for the action functional, then $q(t)$ solves*

$$0 = \frac{\partial S}{\partial t} + H\left(t, q, \frac{\partial S}{\partial q}\right), \tag{6.4}$$

where H is total energy defined by (4.22).

Equation (6.4) is the **Hamilton–Jacobi equation**, and for a system with n degrees of freedom there are $n + 1$ independent variables $(t, q_1, \ldots, q_n)$. It is often the case in practice that the formula for $S(t, q)$ is unknown, and cannot be determined from (6.4) alone.

The solution, or **complete integral**, of this equation has $n + 1$ integration constants corresponding to the number of independent variables. Denoting these constants by $\alpha_1, \ldots, \alpha_n$, and A, we write

$$S = f\left(t, q_1, \ldots, q_n, \alpha_1, \ldots, \alpha_n\right) + A.$$

Indeed, one of these constants must be additive since the action appears in the PDE (6.4) only through its partial derivatives and hence is invariant under the addition of a constant. Mathematically, we require that a complete integral $S(t, q, \alpha)$ to the Hamilton–Jacobi equation (6.4) satisfies

$$\det \frac{\partial^2 S}{\partial q \, \partial \alpha} \neq 0$$

in order to avoid incomplete solutions.

The function $f(t, q_1, \ldots, q_n, \alpha_1, \ldots, \alpha_n)$ induces a change of coordinates. (We will develop this idea more generally in section 7.6, where we will see that f is an example of a generating function which generates a canonical transformation.) Think of $\alpha_1, \ldots, \alpha_n$ as new momenta, and let $\beta_1, \ldots, \beta_n$ denote new coordinates to be chosen. Note that by the chain rule,

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial q} \cdot \dot{q} + \frac{\partial f}{\partial \alpha} \cdot \dot{\alpha}. \tag{6.5}$$

The q_i derivatives are the momenta by (6.1), and we set

$$\beta_i := -\frac{\partial f}{\partial \alpha_i}. \tag{6.6}$$

Consider the new total energy

$$H'(t,\alpha,\beta) := H + \frac{\partial f}{\partial t} = H + \frac{\partial S}{\partial t} = 0,$$

which has corresponding Lagrangian

$$\begin{aligned}\mathscr{L}'(t,\beta,\alpha) := \alpha\cdot\dot\beta - H' = \alpha\cdot\dot\beta &= -\frac{\mathrm{d}f}{\mathrm{d}t} + \frac{\partial f}{\partial t} + \frac{\partial f}{\partial q}\cdot\dot q \\ &= -\frac{\mathrm{d}f}{\mathrm{d}t} - H + p\cdot\dot q = \mathscr{L} - \frac{\mathrm{d}f}{\mathrm{d}t}\end{aligned}$$

by the chain rule (6.5). As this new Lagrangian $\mathscr{L}'$ differs from the old $\mathscr{L}$ by a complete time derivative, then they generate the same motion by Corollary 4.6.

For any Lagrangian $\mathscr{L}$, the definition of the total energy (4.22) requires

$$\begin{aligned}\frac{\partial H}{\partial p} &= \frac{\partial}{\partial p}\left(p\cdot\dot q - \mathscr{L}(t,q,\dot q)\right) = \dot q, \\ \frac{\partial H}{\partial q} &= \frac{\partial}{\partial q}\left(p\cdot\dot q - \mathscr{L}(t,q,\dot q)\right) = -\frac{\partial\mathscr{L}}{\partial q} = -\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathscr{L}}{\partial\dot q} = -\dot p.\end{aligned}$$

This calculation may appear questionable at first: it is not clear that the velocity $\dot q$ is independent of the position q and momentum p. However, it is indeed correct, and we will later give it thorough justification in section 7.1. Applying this to our new total energy $H'(t,\beta,\alpha)$, we observe that

$$\dot\alpha = 0, \quad \dot\beta = 0.$$

In other words, we have used the integration constants α to generate corresponding conserved quantities β. Recalling the definition (6.6) of the coordinates β, we conclude

$$\frac{\partial S}{\partial\alpha_i}(t,q,\alpha) = \text{constant} \tag{6.7}$$

in the n coordinates and time. In fact, even if we can only obtain a partial solution to the Hamilton–Jacobi equation involving only m constants α_i, we still get the corresponding m constants of motion.

Lastly, let us specialize to a conservative system. In this case, the total energy H is equal to a constant E and the action integral becomes

$$\begin{aligned}S(q(t)) &= \int_0^t \mathscr{L}(t,q(t),\dot q(t))\,\mathrm{d}t = \int_0^t \left(p\cdot\dot q - H\right)\,\mathrm{d}t \\ &= \int_0^t p\cdot\dot q\,\mathrm{d}t - \int_0^t E\,\mathrm{d}t = S_0\left(q_1,\dots,q_n\right) - Et,\end{aligned}$$

for some $S_0(q)$ which is only a function of the coordinates. As $\frac{\partial S_0}{\partial t} = 0$, the Hamilton–Jacobi equation then takes the special form

$$H\left(q,\frac{\partial S}{\partial q},t\right) = E. \tag{6.8}$$

In particular, we are no longer required to know the exact formula for the action.

6.2. Separation of variables

Sometimes we can reduce the Hamilton–Jacobi equation by one coordinate using separation of variables. Suppose that for some system with n degrees of freedom, we have a coordinate q_1 with corresponding derivative $\frac{\partial S}{\partial q_1}$ that appear in the Hamilton–Jacobi equation only in some particular combination $\phi(q_1, \frac{\partial S}{\partial q_1})$. That is, the Hamilton–Jacobi equation (6.4) takes the form

$$\Phi\left(t, q_2, \dots, q_n, \frac{\partial S}{\partial q_2}, \dots, \frac{\partial S}{\partial q_n}, \phi\left(q_1, \frac{\partial S}{\partial q_1}\right)\right) = 0 \tag{6.9}$$

after rearranging the independent variables. To look for a solution S, we take the ansatz

$$S = S'(q_2, \dots, q_n, t) + S_1(q_1).$$

Plugging this back into our Hamilton–Jacobi equation (6.9) we get

$$\Phi\left(t, q_2, \dots, q_n, \frac{\partial S'}{\partial q_2}, \dots, \frac{\partial S'}{\partial q_n}, \phi\left(q_1, \frac{\mathrm{d}S_1}{\mathrm{d}q_1}\right)\right) = 0. \tag{6.10}$$

Note that q_1 only influences ϕ and is entirely independent from the rest of the expression. As the variables are independent, this can only happen if ϕ is constant:

$$\phi\left(q_1, \frac{dS_1}{dq_1}\right) = \alpha_1, \quad \Phi\left(t, q_2, \dots, q_n, \frac{\partial S'}{\partial q_2}, \dots, \frac{\partial S'}{\partial q_n}, \alpha_1\right) = 0. \tag{6.11}$$

We now have a first order ODE and a Hamilton–Jacobi equation in terms of the remaining $n - 1$ coordinates. The ability to remove a coordinate in the Hamilton–Jacobi consideration even when it is not cyclic is a virtue of this formulation.

If we do have some cyclic coordinate q_1 for the system (i.e. $\mathscr{L}$ is independent of q_1), then the Hamilton–Jacobi equation (6.4) becomes

$$\frac{\partial S}{\partial t} + H\left(q_2, \dots, q_n, \frac{\partial S}{\partial q_1}, \dots, \frac{\partial S}{\partial q_n}, t\right) = 0. \tag{6.12}$$

Then q_1 is of the type (6.9) for the function

$$\phi\left(q_1, \frac{\partial S}{\partial q_1}\right) = \frac{\partial S}{\partial q_1}. \tag{6.13}$$

Our result (6.11) yields

$$\frac{\partial S}{\partial q_1} = \alpha_1, \quad S = S'(q_2, \dots, q_n, t) + \alpha_1 q_1. \tag{6.14}$$

Here, $\alpha_1 = \partial S/\partial q_1$ is just the conserved momentum corresponding to q_1.

If this cyclic variable is time, then the system is conservative and we saw in (6.8) that the action is given by

$$S = W\left(q_1, \ldots, q_n\right) - Et. \tag{6.15}$$

Here, $-E$ is the conserved quantity associated with t, although it is not necessarily always the total energy. We have used W instead of S' to denote this special case, but they share the same purpose; this W is called **Hamilton's characteristic function**. The Hamilton–Jacobi equation is now

$$H\left(q_1, \ldots, q_n, \frac{\partial W}{\partial q_1}, \ldots, \frac{\partial W}{\partial q_n}\right) = -\frac{\partial S}{\partial t} = E, \tag{6.16}$$

and E is just one integration constant α_j of the motion that does not appear in S'. The corresponding conserved quantity (6.7) will give the coordinates implicitly as functions of the constants α_i, β_i, and time:

$$\beta_i = \frac{\partial S}{\partial \alpha_i} = \begin{cases} \dfrac{\partial W}{\partial \alpha_i} - t & \text{for } i = j, \\ \dfrac{\partial W}{\partial \alpha_i} & \text{for } i \neq j. \end{cases} \tag{6.17}$$

Only the jth of these equations is time-dependent, and so one of the q_i can be chosen as an independent variable and the rest will be able to be written in terms of this coordinate. For example, in section 3.1 we saw that for central forces the angle ϕ can be soled for as a function of the radius r.

6.3. Conditionally periodic motion

For this section, we will examine a system of n degrees of freedom with bounded motion, such that every variable can be separated using the method of the previous section. This means the action takes the form

$$S = \sum_{i=1}^{d} S_i(q_i) + S'(t), \tag{6.18}$$

where each coordinate S_i is related to the corresponding momentum via

$$p_i = \frac{\partial S_i}{\partial q_i}, \qquad S_i = \int p_i \, \mathrm{d}q_i. \tag{6.19}$$

The motion is bounded, and so this integral represents the area enclosed by a loop in the phase plane (q_i, p_i) (just as with the period integral (2.9)). Every time q_i returns to a value, S_i has incremented by an amount $2\pi I_i$ with

$$I_i = \frac{1}{2\pi} \oint p_i \, \mathrm{d}q_i. \tag{6.20}$$

These I_i are called the **action variables**.

As in section 6.1, the function S_i induces a change of variables with the action variables I_i as the new momenta. (Later, we will see that S_i is a generating function that induces a canonical transformation.) The new position coordinates, called **angle variables**, are given by

$$w_i = \frac{\partial S}{\partial I_i} = \sum_{k=1}^{n} \frac{\partial S_k}{\partial I_i}(q_k, I_1, \ldots, I_n) \tag{6.21}$$

since this is the time integral of $\frac{\partial H}{\partial p} = \dot{q}$. The functions S_i are time-independent, and so the new total energy $H \equiv E$ is just the old in terms of the new coordinates. The new equations of motion require

$$\dot{I}_i = -\frac{\partial H}{\partial w_i}(I_1, \ldots, I_n) = 0, \quad \dot{w}_i = \frac{\partial H}{\partial I_i}(I_1, \ldots, I_n) = \frac{\partial E}{\partial I_i}(I_1, \ldots, I_s), \tag{6.22}$$

which can be immediately integrated to yield

$$I_i = \text{constant}, \quad w_i = \frac{\partial E}{\partial I_i} t + \text{constant}. \tag{6.23}$$

As we have already observed, S_i increments by $2\pi I_i$ each time q_i returns to its original value, and so the angle variables w_i also increment by 2π. Consequently the derivative $\frac{\partial E}{\partial I_i}$ is the frequency of motion in the ith coordinate, which *we were able to identify without solving the entire system.*

As the motion in these variables is periodic, any single-valued function $F(q, p)$ of the system coordinates and momenta will be periodic in the angle variables with period 2π after being transformed to the canonical variables. Fourier expanding in each of the angle variables, we have

$$F = \sum_{\ell \in \mathbb{Z}^n} A_\ell e^{i\ell \cdot w} = \sum_{\ell_1, \ldots, \ell_n \in \mathbb{Z}} A_{\ell_1 \ldots \ell_n} e^{i(\ell_1 w_1 + \cdots + \ell_n w_n)}. \tag{6.24}$$

Using (6.23), we may write the angle variables as functions of time. Absorbing the integration constants of the w_i into the coefficients A_ℓ, we get

$$F = \sum_{\ell \in \mathbb{Z}^n} A_\ell \exp\left(it\ell \cdot \frac{\partial E}{\partial I} \right). \tag{6.25}$$

Each term of this sum is periodic with frequency $\ell \cdot \frac{\partial E}{\partial I}$. If the frequencies $\frac{\partial E}{\partial I_i}$ are not commensurable however, then the total quantity F is not periodic. In particular, the coordinates q, p are may not be periodic, and the system may not return to any given state that it instantaneously occupies. However, if we wait long enough the system will come arbitrarily close to any given occupied state—this phenomenon is referred to as *Poincaré's recurrence theorem* (cf. Corollary 7.26). Such motion is called **conditionally periodic**.

Two frequencies $\frac{\partial E}{\partial I_i}$ that are commensurable (i.e. their ratio is a rational number) are called a **degeneracy** of the system, and if all n are commensurable

the system is said to be **completely degenerate**. In the latter case, all motion is periodic, and so we must have a full set of $2n-1$ conserved quantities. Only n of these will be independent, and so they can be defined to be the action variables $I_1, \ldots, I_n$. The remaining $n-1$ constants may be chosen to be $w_i \frac{\partial E}{\partial I_k} - w_k \frac{\partial E}{\partial I_i}$ for distinct i, k, since

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(w_i \frac{\partial E}{\partial I_k} - w_k \frac{\partial E}{\partial I_i}\right) = \dot{w}_i \frac{\partial E}{\partial I_k} - \dot{w}_k \frac{\partial E}{\partial I_i} = \frac{\partial E}{\partial I_i}\frac{\partial E}{\partial I_k} - \frac{\partial E}{\partial I_k}\frac{\partial E}{\partial I_i} = 0.$$

Note, however, that since the angle variables are not single-valued, neither will be the $n-1$ constants of motion.

Consider a partial degeneracy, say, of frequencies 1 and 2. This means

$$k_1 \frac{\partial E}{\partial I_1} = k_2 \frac{\partial E}{\partial I_2} \tag{6.26}$$

for some $k_1, k_2 \in \mathbb{Z}$. The quantity $w_1 k_2 - w_2 k_1$ will then be conserved, since

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(w_1 k_1 - w_2 k_2\right) = \dot{w}_1 k_1 - \dot{w}_2 k_2 = \frac{\partial E}{\partial I_1} k_1 - \frac{\partial E}{\partial I_2} k_2 = 0. \tag{6.27}$$

Note that this quantity is single-valued modulus 2π, and so a trigonometric function of it will be an actual conserved quantity.

In general, for a system with n degrees of freedom whose action is totally separable and has n single-valued integrals of motion, the system state moves densely in a n-dimensional manifold in $2d$-dimensional phase space. For degenerate systems we have more than n integrals of motion, and consequently the system state is confined to a manifold of dimension less than n. When a system has less than n degeneracies, then there has fewer than n integrals of motion and the system state travels within a manifold of dimension greater than n.

6.4. Geometric optics analogy

Hamilton came up with the principle of least action while studying optics, and was inspired by Fermat's optics principle. In this section we will see that the level sets of the action propagate through configuration space mathematically similar to how light travels through a medium. This connection brings a physical analogy to the formerly abstract notion of the action.

Suppose we have a system consisting of one particle moving in the Euclidean space $\mathbb{R}^3$ for which the total energy is conserved. (Although this analogy holds for systems with multiple particles and more complicated configuration spaces, we will focus on this simple case for convenience.) Equation (6.15) tells us that the action is given by

$$S(q,t) = W(q) - Et. \tag{6.28}$$

Take Cartesian coordinates $q = \mathbf{x} = (x, y, z) \in \mathbb{R}^3$, and consider the motion of the action level surfaces $S(t, q) = b$ with time in $\mathbb{R}^3$. (If we were to generalize this argument to multiple-particle systems, then instead of the particle's

motion in Cartesian space we must consider the path that the system traces out in configuration space.) At time $t = 0$, we have an equation for Hamilton's characteristic function $W = b$, and after a time step Δt we then have

$$W(\Delta t) + \Delta W = b + E\Delta t + \mathcal{O}(\Delta t^2)$$

since $\frac{\mathrm{d}W}{\mathrm{d}t} = E$.

The propagation of this surface can be thought of as a wavefront. If we call the distance traveled normal to the wavefront $\mathrm{d}s$, then we also have

$$\frac{\partial W}{\partial s} = |\nabla W|. \tag{6.29}$$

The velocity u of the wavefront is then

$$u = \frac{\mathrm{d}s}{\mathrm{d}t} = \frac{dW/|\nabla W|}{dW/E} = \frac{E}{|\nabla W|}.$$

As a conservative system, the Hamilton–Jacobi equation takes the form (6.16), which in Cartesian coordinates looks like

$$E = H\left(q, \frac{\partial W}{\partial q}\right) = K\left(\frac{\partial W}{\partial q}\right) + V = \frac{(\nabla W)^2}{2m} + V,$$

or after rearranging,

$$(\nabla W)^2 = 2m(E - V). \tag{6.30}$$

Plugging this into the velocity (6.29), we have

$$u = \frac{E}{\sqrt{2m(E-V)}} = \frac{E}{\sqrt{2mK}} = \frac{E}{p}.$$

The faster the particle moves, the slower the action level sets propagate.

The momentum is given by

$$p = \frac{\partial W}{\partial q} = \nabla W.$$

The gradient is of course normal to the level sets, and so this relation tells us that the particle always moves normal to the level sets of the characteristic function W.

We will now see how the level sets of the action propagate like waves. For some scalar-valued function ϕ, the wave equation of optics is

$$\nabla^2\phi - \frac{n^2}{c^2}\frac{\partial^2\phi}{\partial t^2} = 0. \tag{6.31}$$

If the refractive index n is constant, then there is a family of plane wave solutions:

$$\phi(t, r) = \phi_0 e^{i(\mathbf{k}\cdot\mathbf{x} - \omega t)}, \tag{6.32}$$

where the vector $\mathbf{k} \in \mathbb{R}^3$ is the propagation direction and the magnitude of $k = \frac{2\pi}{\lambda} = \frac{n\omega}{c}$ is the **wave number**.

In geometric optics, the refractive index $n \equiv n(\mathbf{x})$ is not assumed to be constant, but rather to be changing slowly on the scale of the wavelength. Consequentially, we now seek solutions to the wave equation (6.31) with the ansatz based on the plane waves (6.32):

$$\phi(t, r) = e^{A(\mathbf{x}) + ik_0(L(\mathbf{x}) - ct)}. \tag{6.33}$$

where $A(\mathbf{x})$ is related to the amplitude of the wave, $k_0 = \frac{\omega}{c}$ is the wave number in vacuum ($n \equiv 1$), and $L(\mathbf{x})$ is called the **optical path length** of the wave. Plugging in (6.33), the wave equation (6.31) becomes

$$\phi \left\{ \left[\nabla^2 A + (\nabla A)^2 - k_0^2 (\nabla L)^2 + k_0^2 n^2 \right] + ik_0 \left[\nabla^2 L + 2\nabla A \cdot \nabla L \right] \right\} = 0.$$

In general, ϕ is nonzero and so the curly-bracketed expression must vanish. We want A and L to be real-valued by construction, and so we the real and imaginary parts in square brackets must also vanish:

$$\nabla^2 A + (\nabla A)^2 + k_0^2 \left[n^2 - (\nabla L)^2 \right] = 0, \quad \nabla^2 L + 2\nabla A \cdot \nabla L = 0. \tag{6.34}$$

Now comes the geometric optics approximation: the wavelength $\lambda = \frac{2\pi}{k}$ is small compared to the rate of change of the medium. In particular, the wave number in vacuum $k_0 = \frac{2\pi}{\lambda_0}$ must be considerably large compared to the derivative terms in the first equation of (6.34), and thus we require

$$(\nabla L)^2 = n^2.$$

This is called the **eikonal equation**.

Returning to (6.30), we see that the characteristic function W satisfies an eikonal equation for a "medium" of refractive index $\sqrt{2m(E - V)} = p$ (this equality holds for the single-particle case). This illustrates that the characteristic function is like a wavefront that propagates through the medium of configuration space with refractive index p, in the geometric optics approximation.

6.5. Exercises

6.1 (Harmonic oscillator)**.** The harmonic oscillator has total energy

$$H = \tfrac{1}{2m} p^2 + \tfrac{1}{2} m\omega^2 q^2.$$

(a) Write down the Hamilton–Jacobi equation (6.4) for this system. As this system is conservative, we expect a solution (up to an arbitrary additive constant) of the form

$$S(q, \alpha, t) = W(q, \alpha) - \alpha t$$

where the constant α is the total energy. Plug this ansatz into the Hamilton–Jacobi equation and conclude that

$$W = \pm m\omega \int \sqrt{\tfrac{2\alpha}{m\omega^2} - q^2}\, \mathrm{d}q.$$

This integral can be evaluated further, but it is not necessary for our purposes.

(b) The quantity β will implicitly give us the equation of motion $q(\alpha, \beta, t)$. Using the definition (6.6), show that

$$t + \beta = \frac{1}{\omega} \begin{Bmatrix} \sin^{-1}\left(\sqrt{\frac{m}{2\alpha}}\omega q\right) & \text{if } \pm = + \\ \cos^{-1}\left(\sqrt{\frac{m}{2\alpha}}\omega q\right) & \text{if } \pm = - \end{Bmatrix} + \text{constant}.$$

Note that we may assume that we are in the case $\pm = -$ and absorb the integration constant into β, which has yet to be determined. Altogether, this yields the familiar equation of motion

$$q(t) = \sqrt{\tfrac{2\alpha}{m\omega^2}} \cos\left[\omega(t + \beta)\right].$$

(c) To find the constants we must apply the initial conditions $q(0) = q_0$, $p(0) = p_0$. Determine α and β using $p_0 = \frac{\partial S}{\partial q}|_{t=0}$ and $q(0) = q_0$ respectively, and obtain the solution as a function of the initial values:

$$q(t) = \sqrt{q_0^2 + \frac{p_0^2}{m^2\omega^2}} \cos\left[\omega t + \cos^{-1}\left(\frac{q_0}{\sqrt{q_0^2 + \frac{p_0^2}{m^2\omega^2}}}\right)\right].$$

6.2 (Central field)**.** Consider the motion of a particle in a central field as in section 3.1. In polar coordinates, we have

$$\begin{gathered} K = \tfrac{m}{2}(\dot{r}^2 + r^2\dot{\phi}^2), \quad V = V(r), \\ p_r = \frac{\partial \mathscr{L}}{\partial \dot{r}} = m\dot{r}, \quad p_\phi = \frac{\partial \mathscr{L}}{\partial \dot{\phi}} = mr^2\dot{\phi}, \\ H = \tfrac{1}{2m}(p_r^2 + r^{-2}p_\phi^2) + V(r). \end{gathered}$$

(a) This total energy is both time-independent and cyclic in ϕ, and so we expect an action of the form

$$S = W_1(r) + \alpha_\phi \phi - Et.$$

Plug this into the Hamilton–Jacobi equation (6.16) for conservative systems and integrate to arrive at

$$W = W_1(r) + \alpha_\phi \phi = \pm \int \sqrt{2m(E - V(r)) - \alpha_\phi^2 r^{-2}}\, \mathrm{d}r + \alpha_\phi \phi.$$

(b) Use (6.17) to obtain the implicit equations of motion

$$\beta_1 = \pm \int \frac{m}{\sqrt{2m(E - V(r)) - \alpha_\phi^2 r^{-2}}} \, \mathrm{d}r - t,$$
$$\beta_2 = \pm \int \frac{-\alpha_\phi r^{-2}}{\sqrt{2m(E - V(r)) - \alpha_\phi^2 r^{-2}}} \, \mathrm{d}r + \phi.$$

These match what we found in equations (3.5) and (3.6) where $\alpha_\phi = M$ is the angular momentum, which is the constant associated to the cyclic coordinate ϕ.

6.3 (Kepler's problem)**.** We will find the frequency of oscillations for Kepler's problem using action variables without solving the equations of motion. Consider a particle of mass m in an inverse-square central force field, as in section 3.3:

$$K = \tfrac{m}{2}(\dot{r}^2 + r^2\dot{\theta}^2 + r^2 \sin^2\theta \dot{\phi}^2), \quad V = -kr^{-1},$$
$$p_r = \frac{\partial \mathscr{L}}{\partial \dot{r}} = m\dot{r}\ , \quad p_\theta = \frac{\partial \mathscr{L}}{\partial \dot{\theta}} = mr^2\dot{\theta}, \quad p_\phi = \frac{\partial \mathscr{L}}{\partial \dot{\phi}} = mr^2 \sin^2\theta \dot{\phi},$$
$$H = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 \sin^2\theta}\right) - \frac{k}{r}.$$

The constant k is positive, so that we have an attractive force in order to have bounded motion.

(a) Write down the Hamilton–Jacobi equation (6.16) for this conservative system. Notice that all of the coordinates are separable, and so the characteristic function is of the form

$$W = W_r(r) + W_\theta(\theta) + W_\phi(\phi).$$

(b) The total energy is cyclic in ϕ and thus has constant $\frac{\partial W}{\partial \phi} = \frac{\partial W_\phi}{\partial \phi} = \alpha_\phi$, which is angular momentum about the z-axis. Plug this in, group the terms involving only θ and conclude that

$$\left(\frac{\partial W_\theta}{\partial \theta}\right)^2 + \frac{\alpha_\phi^2}{\sin^2\theta} = \alpha_\theta^2, \quad \frac{1}{2m}\left[\left(\frac{\partial W_r}{\partial r}\right)^2 + \frac{\alpha_\theta^2}{r^2}\right] - \frac{k}{r} = E.$$

The equations for W_ϕ, W_θ, and W_r demonstrate the conservations of angular momentum about the z-axis p_θ, total angular momentum p, and total energy E, and from here they could be integrated to obtain the equations of motion.

(c) Use the three differential equations of part (b) to obtain the action variables:

$$\begin{aligned} I_\phi &= \alpha_\phi = p_\phi, \\ I_\theta &= \frac{1}{2\pi} \oint \sqrt{\alpha_\theta^2 - \frac{\alpha_\phi^2}{\sin^2\theta}}\, \mathrm{d}\theta, \\ I_r &= \frac{1}{2\pi} \oint \sqrt{2mE + \frac{2mk}{r} - \frac{\alpha_\theta^2}{r^2}}\, \mathrm{d}r. \end{aligned}$$

(d) Let us look at the second action variable I_θ. We know from section 3.1 that this motion is coplanar, so let ψ denote the angle in the plane of orbit. Set the momentum in the (r, θ, ϕ) variables and (r, ψ) variables equal, and conclude that $p_\theta\, \mathrm{d}\theta = p\, \mathrm{d}\psi - p_\phi\, \mathrm{d}\phi$. Conclude that

$$I_\theta = p - p_\phi = \alpha_\theta - \alpha_\phi.$$

(e) Now for the third action variable I_r. The integral for I_r is evaluated between two turning points r_1, r_2 for which the integrand $p_r = m\dot{r}$ must vanish. We can therefore integrate from r_2 to r_1 and back to r_2, for which the integrand is first negative then positive, corresponding to the sign of the momentum $p_r = m\dot{r}$. In the complex plane, this integrand is analytic everywhere but $r = 0$ and along the segment on the real axis connecting r_1 and r_2. Integrate around a counterclockwise contour enclosing r_1 and r_2 to obtain

$$I_r = -\alpha_\theta^2 + \frac{mk}{\sqrt{-2mE}} = -(I_\theta + I_\phi) + \frac{mk}{\sqrt{-2mE}}.$$

Note that the energy

$$E(I) = -\frac{mk^2}{2(I_r + I_\theta + I_\phi)^2}$$

is symmetric in the three action variables, and so the frequency of oscillations in each coordinate r, θ, ϕ is the same:

$$\frac{\partial E}{\partial I_r} = \frac{\partial E}{\partial I_\theta} = \frac{\partial E}{\partial I_\phi} = \frac{mk^2}{(I_r + I_\theta + I_\phi)^3}.$$

This agrees with the fact that the force is rotationally symmetric.

PART III

HAMILTONIAN MECHANICS

Hamiltonian mechanics treats the position and momentum variables as independent coordinates on phase space. This yields Hamilton's equations of motion—a system with two first-order differential equations for each degree of freedom—which portrays the system's motion as the flow of a particular vector field on phase space. While we are still free to choose coordinates, the position and momentum variables are of course not truly independent quantities, and consequently permissible changes of variables must preserve the class of such vector fields. This underlying structure of these vector fields induces a geometry on phase space, which is the foundation of symplectic and contact structures in differential geometry.

CHAPTER 7

HAMILTON'S EQUATIONS

In this chapter we will develop Hamilton's equations and Poisson structure on Euclidean space. The material for this chapter is based on [MZ05], [Arn89, Ch. 3], [Gol51, Ch. 7–8], and [LL76, Ch. 7].

7.1. Hamilton's equations

A conservative system in Euclidean space with n degrees of freedom obeys Newton's equation (1.3), which reads

$$\dot{\mathbf{p}} = -\nabla V(\mathbf{x}).$$

Here, we have $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_N) \in \mathbb{R}^n$ and $\mathbf{p}_i = m_i \mathbf{x}_i$, which makes this a second-order equation in $\mathbf{x}$. We can recast this as the first-order system

$$\dot{\mathbf{x}}_i = \tfrac{1}{m_i}\mathbf{p}_i, \qquad \dot{\mathbf{p}} = -\nabla V(\mathbf{x}).$$

In terms of the system's total energy

$$E(\mathbf{x}, \mathbf{p}) = \sum_{i=1}^{N} \tfrac{1}{2m_i}|\mathbf{p}_i|^2 + V(\mathbf{x}),$$

this takes the particularly simple form

$$\dot{\mathbf{x}} = \frac{\partial E}{\partial \mathbf{p}}, \qquad \dot{\mathbf{p}} = -\frac{\partial E}{\partial \mathbf{x}}. \tag{7.1}$$

In this way, the total energy induces the flow of $(\mathbf{x}(t), \mathbf{p}(t))$ on the phase space $\mathbb{R}^{2n}$.

Now suppose we start with a smooth function $H(t, q, p)$ on $\mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n$. In the spirit of (7.1), we define **Hamilton's equations of motion**

$$\dot{q} = \frac{\partial H}{\partial p}, \qquad \dot{p} = -\frac{\partial H}{\partial q} \tag{7.2}$$

for the **Hamiltonian** $H(t, q, p)$. In particular, if H is the total energy $E(\mathbf{x}, \mathbf{p})$ of a conservative system on $\mathbb{R}^n$, then (7.1) shows that Hamilton's equations (7.2) implies Newton's equations (1.3).

Next, we will show that given a Hamiltonian, Hamilton's equations are equivalent to Lagrange's equations for the corresponding Lagrangian. In section 7.2, we will see how to transform a Lagrangian into a Hamiltonian, and so together this will complete the equivalence of Hamiltonian and Lagrangian mechanics.

Proposition 7.1 (Principle of least action)**.** *The path $(p(t), q(t))$ is a critical point for the functional*

$$S(p(t), q(t)) = \int_0^T \left[\sum_{i=1}^n p_i(t)\dot{q}_i(t) - H(p(t), q(t)) \right] dt \tag{7.3}$$

over fixed-endpoint variations if and only if $(p(t), q(t))$ solves Hamilton's equations (7.2)*.*

Heuristically, we can write the action integral (7.3) as

$$S = \int (p\,\mathrm{d}q - H\,\mathrm{d}t).$$

We will revisit this interpretation in section 9.5 (cf. (9.16)).

Proof. Consider $p(t) + \epsilon\phi(t)$ and $q(t) + \epsilon\psi(t)$ with ϕ, ψ smooth $\mathbb{R}^n$-valued functions satisfying $\psi(0) = 0 = \psi(T)$. Then

$$\begin{aligned} 0 &= \frac{\mathrm{d}}{\mathrm{d}\epsilon} S(p + \epsilon\phi, q + \epsilon\psi)\bigg|_{\epsilon=0} \\ &= \int_0^T \sum_{i=1}^n \left[\phi_i \dot{q}_i + p_i \dot{\psi}_i - \frac{\partial H}{\partial p_i}\phi_i - \frac{\partial H}{\partial q_i}\psi_i \right] \mathrm{d}t \\ &= \left[p\psi\right]_{t=0}^{t=T} + \int_0^T \phi \left[\dot{q} - \frac{\partial H}{\partial p} \right] \mathrm{d}t + \int_0^T \left[-\dot{p} - \frac{\partial H}{\partial q} \right] \mathrm{d}t. \end{aligned}$$

The first term on the RHS vanishes as $\psi(0) = 0 = \psi(T)$. In order for this to vanish for all such ϕ, ψ, we must have that Hamilton's equations (7.2) hold. □

Next we will see how conservation of momentum and energy are manifested in the Hamiltonian perspective. A position variable q_k is **cyclic** if the Hamiltonian H is independent of q_k (but may depend on p_k). For such a variable, the corresponding component of Hamilton's equations (7.2) reads

$$\dot{q}_k = \frac{\partial H}{\partial p_k}, \qquad \dot{p}_k = 0. \tag{7.4}$$

The second of these equations expresses the conservation of p_k, which we record in the following statement:

Proposition 7.2 (Conservation of momentum)**.** *If the Hamiltonian is independent of a position variable q_k (but possibly dependent on p_k), then the corresponding momentum p_k is conserved.*

The first equation of (7.4) is then independent of q_k and is thus can be directly integrated. In this way, we are left with $2n-2$ equations in terms of the integration constant p_k.

When time is the cyclic coordinate, the corresponding conserved quantity is the Hamiltonian:

Proposition 7.3 (Conservation of energy)**.** *If the Hamiltonian H is independent of time t, then H is conserved.*

Proof. The chain rule yields

$$\frac{\mathrm{d}}{\mathrm{d}t}H(q(t),p(t)) = \frac{\partial H}{\partial q}\cdot\dot{q} + \frac{\partial H}{\partial p}\cdot\dot{p} = \frac{\partial H}{\partial q}\cdot\frac{\partial H}{\partial p} - \frac{\partial H}{\partial p}\cdot\frac{\partial H}{\partial q} = 0,$$

where in the second equality we used that $q(t)$ and $p(t)$ solve Hamilton's equations (7.2). □

7.2. Legendre transform

The Legendre transform is an involution on the space of strictly convex functions, which provides a correspondence between the Lagrangian and Hamiltonian perspectives. Specifically, Lagrangians and Hamiltonians are often strictly convex in $\dot{q}$ and p due to the quadratic kinetic energy term, and they are Legendre transforms of each other in in those variables.

Let $f:\mathbb{R}^n\to\mathbb{R}$ be a smooth, nonnegative, strictly convex function with $f(0)=0$ that satisfies $f(\mathbf{x})/|\mathbf{x}|\to+\infty$ as $|\mathbf{x}|\to\infty$. We define

$$f^*(\boldsymbol{\xi}) = \sup_{\mathbf{x}\in\mathbb{R}^n}\{\mathbf{x}\cdot\boldsymbol{\xi} - f(\mathbf{x})\} \tag{7.5}$$

to be the **Legendre transform** of $f(\mathbf{x})$. Inside the supremum is the distance $F(\mathbf{x},\boldsymbol{\xi}) = \mathbf{x}\cdot\boldsymbol{\xi} - f(\mathbf{x})$ between the graph of the function $f(\mathbf{x})$ and the hyperplane $\mathbf{x}\cdot\boldsymbol{\xi}$ of slope $\boldsymbol{\xi}$. As $f(\mathbf{x})/|\mathbf{x}|\to+\infty$ as $|\mathbf{x}|\to\infty$, then for fixed $\boldsymbol{\xi}$ the function $\mathbf{x}\mapsto F(\mathbf{x},\boldsymbol{\xi})$ must attain its maximum. Moreover, as f is strictly convex, then $\mathbf{x}\mapsto F(\mathbf{x},\boldsymbol{\xi})$ is strictly concave and so there is a unique point $\mathbf{x}^*(\xi)$ which maximizes $F(\mathbf{x},\boldsymbol{\xi})$. The Legendre transform of f is then given by $f^*(\xi) = F(\mathbf{x}^*(\boldsymbol{\xi}),\boldsymbol{\xi})$.

In the context of classical mechanics, we will be primarily concerned with the application of the Legendre transform to positive definite quadratic functions.

Example 7.4. Consider the quadratic function

$$f(\mathbf{x}) = \tfrac{1}{2}A\mathbf{x}\cdot\mathbf{x} + \mathbf{b}\cdot\mathbf{x} + c,$$

where A is an $n\times n$ real symmetric positive definite matrix, $\mathbf{b}\in\mathbb{R}^n$, and $c\in\mathbb{R}$. In order to maximize the distance $F(\mathbf{x},\boldsymbol{\xi})$, we differentiate:

$$0 = \frac{\partial F}{\partial\mathbf{x}}(\mathbf{x}^*) = \frac{\partial}{\partial\mathbf{x}}\left[\mathbf{x}\cdot\boldsymbol{\xi} - \tfrac{1}{2}A\mathbf{x}\cdot\mathbf{x} - \mathbf{b}\cdot\mathbf{x} - c\right]_{\mathbf{x}=\mathbf{x}^*} = \boldsymbol{\xi} - A\mathbf{x}^* - \mathbf{b}.$$

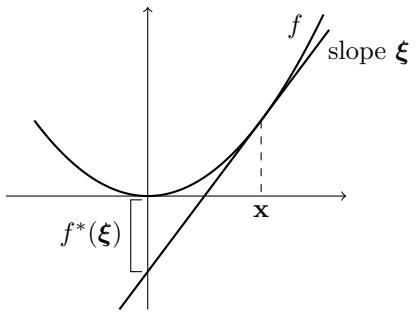


Figure 7.1: Graphically, $f^*(\boldsymbol{\xi})$ is the distance of the origin to the y-intercept of the supporting hyperplane to the graph of $f(\mathbf{x})$ with slope $\boldsymbol{\xi}$.

This equation has one critical point $\mathbf{x}^* = A^{-1}(\boldsymbol{\xi} - \mathbf{b})$, which must be our maximum. Plugging this back in, we get

$$\begin{aligned} f^*(\boldsymbol{\xi}) &= F(\mathbf{x}^*(\boldsymbol{\xi}), \boldsymbol{\xi}) \\ &= A^{-1}(\boldsymbol{\xi} - \mathbf{b}) \cdot \boldsymbol{\xi} - \tfrac{1}{2}(\boldsymbol{\xi} - \mathbf{b}) \cdot A^{-1}(\boldsymbol{\xi} - \mathbf{b}) - \mathbf{b} \cdot A^{-1}(\boldsymbol{\xi} - \mathbf{b}) - c \\ &= \tfrac{1}{2} A^{-1}(\boldsymbol{\xi} - \mathbf{b}) \cdot (\boldsymbol{\xi} - \mathbf{b}) - c. \end{aligned}$$

In particular, if we take $A = mI$, $\mathbf{b} = 0$, and $c = 0$, then both

$$f(\mathbf{x}) = \tfrac{1}{2} m |\mathbf{x}|^2, \qquad f^*(\boldsymbol{\xi}) = \tfrac{1}{2m} |\boldsymbol{\xi}|^2$$

are the kinetic energy once we recognize $\mathbf{x}$ as the velocity and $\boldsymbol{\xi}$ as the momentum.

The Legendre transform can be defined more generally (cf. Exercise 7.3), but with these hypotheses on f we have that f^* satisfies the same hypotheses (although they are not in one-to-one correspondence):

Theorem 7.5 (Involution property)**.** *If $f : \mathbb{R}^n \to \mathbb{R}$ is a smooth, nonnegative, strictly convex function with $f(0) = 0$ that satisfies $f(\mathbf{x})/|\mathbf{x}| \to +\infty$ as $|\mathbf{x}| \to \infty$, then the Legendre transform* (7.5) *is too and we have $(f^*)^* = f$.*

Proof. It is immediate that f^* is nonnegative and that $f^*(0) = 0$. Moreover, f^* convex as the supremum of over convex (indeed, $F(\mathbf{x}, \boldsymbol{\xi})$ is affine in $\boldsymbol{\xi}$) functions.

Next we differentiate $g := f^*$. As the unique maximizer of the distance $F(\mathbf{x}, \boldsymbol{\xi})$, we know that $\mathbf{x}^* = \mathbf{x}^*(\boldsymbol{\xi})$ is the unique solution to

$$0 = \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x}^*) = \xi - \nabla f(\mathbf{x}^*).$$

The function ∇f is a local diffeomorphism on $\mathbb{R}^n$ by the inverse function theorem, since $(\nabla f)' = f''$ is positive definite and hence invertible. This means that the above equation has a unique solution

$$\mathbf{x}^*(\boldsymbol{\xi}) = (\nabla f)^{-1}(\boldsymbol{\xi}) \tag{7.6}$$

which is smooth because ∇f is, and hence $g(\boldsymbol{\xi}) = F(\mathbf{x}^*(\boldsymbol{\xi}), \boldsymbol{\xi})$ is smooth as well. The inverse function theorem also tells us that the derivative of $\mathbf{x}^*(\boldsymbol{\xi})$ is

$$\nabla \mathbf{x}^*(\boldsymbol{\xi}) = (f'')^{-1}(\boldsymbol{\xi})$$

where $f''(\mathbf{x})$ is the Hessian matrix of second derivatives. The first derivative of $g(\boldsymbol{\xi}) := f^*(\boldsymbol{\xi})$ is then

$$\begin{aligned} \nabla g(\boldsymbol{\xi}) &= \nabla \left\{ \boldsymbol{\xi} \cdot \mathbf{x}^*(\boldsymbol{\xi}) - f(\mathbf{x}^*(\boldsymbol{\xi})) \right\} \\ &= \mathbf{x}^*(\boldsymbol{\xi}) + \boldsymbol{\xi} \cdot \nabla \mathbf{x}^*(\boldsymbol{\xi}) - \nabla f(\mathbf{x}^*(\boldsymbol{\xi})) \cdot \nabla \mathbf{x}^*(\boldsymbol{\xi}) = \mathbf{x}^*(\boldsymbol{\xi}). \end{aligned} \tag{7.7}$$

Therefore, the second derivative of g is

$$g''(\boldsymbol{\xi}) = (f'')^{-1}(\boldsymbol{\xi}) > 0,$$

which is positive definite since $f''(\mathbf{x})$ is. That is, the Legendre transform $f^* = g$ is also strictly convex.

Now that we know

$$g(\boldsymbol{\xi}) = \mathbf{x}^*(\boldsymbol{\xi}) \cdot \boldsymbol{\xi} - f(\mathbf{x}^*(\boldsymbol{\xi}))$$

is also convex, we may now consider its Legendre transform. Let $\xi^*(\mathbf{x})$ be the point which attains the supremum for g^*. By (7.6) this point is uniquely determined by

$$\boldsymbol{\xi}^*(\mathbf{x}) = (\nabla g)^{-1}(\mathbf{x}) = \nabla f(\mathbf{x}),$$

where in the last equality we used (7.7). Comparing this with (7.6), we see that his is the inverse of the function $\mathbf{x}^*(\boldsymbol{\xi})$. Consequently, the transform of $g(\boldsymbol{\xi})$ is given by

$$\begin{aligned} g^*(\mathbf{x}) &= \boldsymbol{\xi}^*(\mathbf{x}) \cdot \mathbf{x} - g(\boldsymbol{\xi}^*(\mathbf{x})) \\ &= \boldsymbol{\xi}^*(\mathbf{x}) \cdot \mathbf{x} - \mathbf{x}^*(\boldsymbol{\xi}^*(\mathbf{x})) \cdot \boldsymbol{\xi}^*(\mathbf{x}) + f(\mathbf{x}^*(\boldsymbol{\xi}^*(\mathbf{x}))) = f(\mathbf{x}), \end{aligned}$$

and so $(f^*)^* = f$ as desired. □

Within the context of mechanics, the importance of the Legendre transform is contained in the following simple calculation:

Proposition 7.6. *Let M be an $n \times n$ positive definite matrix. The Legendre transformation of the conservative Lagrangian system*

$$\mathscr{L}(q, \dot{q}) = \tfrac{1}{2} M \dot{q} \cdot \dot{q} - V(q)$$

in $\dot{q}$ is the corresponding Hamiltonian

$$H(q, p) = \tfrac{1}{2} M^{-1} p \cdot p + V(q)$$

in p, and vice versa.

Proof. Apply Example 7.4 to $A = M$, $\mathbf{b} = 0$, and $c = V(q)$ (which is constant with respect to the velocity $\dot{q}$). □

Given a Hamiltonian system, we saw in Proposition 7.1 that the corresponding Lagrangian is given by (7.3) and that Hamilton's equations are equivalent to the principle of least action. Now, given a Lagrangian system, by Proposition 7.6 we see that the corresponding Hamiltonian is given by its Legendre transform:

$$H(q,p,t) := \dot{q}\cdot p - \mathscr{L}(q,\dot{q},t) = \sum_{i=1}^{n} \dot{q}_i \frac{\partial \mathscr{L}}{\partial \dot{q}_i} - \mathscr{L}.$$

Recall that in Proposition 4.11 we saw that the Hamiltonian determines the system's motion, and that the quantity H is conserved whenever the Lagrangian $\mathscr{L}$ is time-independent.

We also see from Proposition 7.6 that the velocity $\dot{q}$ and the momentum p are dual variables. This is encoded in the dot product $\dot{q}\cdot p$ in the definition (7.5), which is also twice the kinetic energy. As the velocity $\dot{q}$ is a tangent vector, then the momentum p must be a covector and so the Hamiltonian is defined on the cotangent bundle of phase space.

7.3. Poisson structure

Unlike the principle of least action, Hamilton's equations (7.2) depend on the choice of coordinates. In this section, we will see that the Poisson bracket provides a coordinate-free reformulation of Hamilton's equations.

Rather than just the position and momentum, let us now consider the evolution of a general observable. If $\mathbf{x}(t)$ evolves according to the first-order ODE system

$$\dot{\mathbf{x}} = \mathbf{f}(t,\mathbf{x}),$$

an **observable** (resp. **time-dependent observable**) is a smooth function F from $\mathbb{R}^d_{\mathbf{x}}$ (resp. $\mathbb{R}_t \times \mathbb{R}^d_{\mathbf{x}}$) into $\mathbb{R}$. The **complete** or **material derivative** of a time-dependent observable F is then

$$\frac{\mathrm{d}}{\mathrm{d}t} F(t,\mathbf{x}) = \frac{\partial F}{\partial t} + \nabla F \cdot \mathbf{f} \tag{7.8}$$

by the chain rule. Note that in addition to the explicit time dependence of F, the evolution of F is influenced by the **advection term** $\mathbf{f}\cdot\nabla F$.

Here, our coordinates $\mathbf{x}$ are $(q,p) \in \mathbb{R}^{2n}$, which evolve under Hamilton's equations. Specifically, by the chain rule and Hamilton's equations (7.2) the material derivative of a time-dependent observable $F(t,q,p)$ is

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \frac{\partial F}{\partial t} + \frac{\partial F}{\partial q}\cdot\dot{q} + \frac{\partial F}{\partial p}\cdot\dot{p} = \frac{\partial F}{\partial t} + \frac{\partial F}{\partial q}\cdot\frac{\partial H}{\partial p} - \frac{\partial F}{\partial p}\cdot\frac{\partial H}{\partial q}. \tag{7.9}$$

Given two time-dependent observables F and H, we define the **(canonical) Poisson bracket** to be the advection term above, i.e.

$$\{F,H\} = \frac{\partial F}{\partial q}\cdot\frac{\partial H}{\partial p} - \frac{\partial F}{\partial p}\cdot\frac{\partial H}{\partial q} = \sum_{k=1}^{n}\left(\frac{\partial F}{\partial q_k}\frac{\partial H}{\partial p_k} - \frac{\partial F}{\partial p_k}\frac{\partial H}{\partial q_k}\right). \tag{7.10}$$

(Note that there is another popular convention with F and H swapped, or equivalently with an overall factor of -1.) Then from (7.9) we see that the material derivative is given by

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \frac{\partial F}{\partial t} + \{F, H\}. \tag{7.11}$$

In particular, if $F(q, p)$ is just a usual observable (i.e. time-independent), then F is conserved by the flow of the Hamiltonian H if and only if $\{F, H\} = 0$.

The evolution (7.11) of observables in terms of the Poisson bracket can be taken as alternative equations of motion. Indeed, (7.11) implies Hamilton's equations (7.2) by taking the observable F to be a position or momentum coordinate:

$$\dot{q}_i = \{q_i, H\} = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = \{p_i, H\} = -\frac{\partial H}{\partial q_i}.$$

As a side note, the equation of motion (7.11) has the added benefit that it is analogous to the Heisenberg formulation of quantum mechanics, where Poisson brackets are replaced by operator commutators.

Next, we record some properties of the Poisson bracket. It is easy to see that the Poisson bracket is bilinear (i.e. linear in each entry) and antisymmetric ($\{F, G\} = -\{G, F\}$) from the definition (7.10). The bracket also posses a product (or Leibniz) rule,

$$\{FG, H\} = F\{G, H\} + G\{F, H\},$$

which can be seen by using the product rule for FG and expanding. We also have the chain rule

$$\{F, g(H)\} = g'(H)\{F, H\}. \tag{7.12}$$

Although slightly less obvious, we claim that the Poisson bracket also satisfies the **Jacobi identity**:

$$\{F, \{G, H\}\} + \{G, \{H, F\}\} + \{H, \{F, G\}\} = 0. \tag{7.13}$$

Let's focus on one of the terms above, say, $\{H, \{F, G\}\}$. As $\{F, G\}$ is a linear expression in terms of the first derivatives of F and G, then $\{H, \{F, G\}\}$ is also linear expression with each term containing exactly one second derivative of F or G. Let $D_G(\phi) = \{G, \phi\}$ and $D_H(\phi) = \{H, \phi\}$. Note that the first term of (7.13) does not contain any second derivatives of F, and so all of the second derivatives of F are contained within

$$\begin{aligned}\{G, \{H, F\}\} + \{H, \{F, G\}\} &= \{G, \{H, F\}\} - \{H, \{G, F\}\} \\ &= (D_G D_H - D_H D_G)F.\end{aligned}$$

To simplify notation and observe some cancellation, we write the operators D_G

and D_H as

$$D_G = \sum_j \left(\frac{\partial G}{\partial p_j}\frac{\partial}{\partial q_j} - \frac{\partial G}{\partial q_j}\frac{\partial}{\partial p_j} \right) = \sum_k \xi_k \frac{\partial}{\partial x_k},$$
$$D_H = \sum_j \left(\frac{\partial H}{\partial p_j}\frac{\partial}{\partial q_j} - \frac{\partial H}{\partial q_j}\frac{\partial}{\partial p_j} \right) = \sum_k \eta_k \frac{\partial}{\partial x_k},$$

where $x = (q, p)$, $\xi = (\frac{\partial G}{\partial p}, -\frac{\partial G}{\partial q})$, and $\eta = (\frac{\partial H}{\partial p}, -\frac{\partial H}{\partial q})$. Therefore

$$D_G D_H = \sum_k \xi_k \frac{\partial}{\partial x_k}\left(\sum_\ell \eta_\ell \frac{\partial}{\partial x_\ell} \right) = \sum_{k,\ell} \left(\xi_\ell \frac{\partial \eta_\ell}{\partial x_k}\frac{\partial}{\partial x_\ell} + \xi_k \eta_\ell \frac{\partial^2}{\partial x_k \partial x_\ell} \right),$$
$$D_H D_G = \sum_k \eta_k \frac{\partial}{\partial x_k}\left(\sum_\ell \xi_\ell \frac{\partial}{\partial x_\ell} \right) = \sum_{k,\ell} \left(\eta_k \frac{\partial \xi_\ell}{\partial x_k}\frac{\partial}{\partial x_\ell} + \eta_k \xi_\ell \frac{\partial^2}{\partial x_k \partial x_\ell} \right).$$

In taking the difference of these, we see that the second terms in these last equalities cancel and we are left with

$$D_G D_H - D_H D_G = \sum_{k,\ell} \left(\xi_k \frac{\partial \eta_\ell}{\partial x_k} - \eta_k \frac{\partial \xi_\ell}{\partial x_k} \right) \frac{\partial}{\partial x_\ell}.$$

That is, all of the second derivatives of F cancel, leaving only first derivatives. By symmetry this must also be true for G and H, and since every term of (7.13) contains only terms containing exactly one second derivative, then all the terms must cancel.

In order to make the equation of motion (7.11) entirely coordinate-free, we need a new coordinate-free definition of the Poisson bracket. Specifically, out of the properties we just observed, we take the following as an abstract definition:

Definition 7.7. A **Poisson bracket** or **Poisson structure** on $\mathbb{R}^d$ is a function $\{\cdot,\cdot\} : C^\infty(\mathbb{R}^d) \times C^\infty(\mathbb{R}^d) \to C^\infty(\mathbb{R}^d)$ satisfying:

(a) (Antisymmetry) $\{F, G\} = -\{G, F\}$ for all $F, G \in C^\infty(\mathbb{R}^d)$.

(b) (Bilinearity) $\{\lambda F + \mu G, H\} = \lambda\{F, H\} + \mu\{G, H\}$ for all $F, G, H \in C^\infty(\mathbb{R}^d)$ and $\lambda, \mu \in \mathbb{R}$.

(c) (Product rule) $\{FG, H\} = \{F, H\}G + F\{G, H\}$ for all $F, G, H \in C^\infty(\mathbb{R}^d)$.

(d) (Jacobi identity) $\{\{F, G\}, H\} + \{\{G, H\}, F\} + \{\{H, F\}, G\} = 0$ for all $F, G, H \in C^\infty(\mathbb{R}^d)$.

We also say that a Poisson bracket is **nondegenerate** if $\nabla F(x) \neq 0$ implies that there exists $G \in C^\infty(\mathbb{R}^d)$ so that $\{F, G\}(x) \neq 0$.

In fact, this definition can even be generalized to manifolds. However, we choose to focus on the Euclidean case for clarity; we will consider general manifolds when we develop symplectic geometry.

Recall the following fact from differential geometry (e.g. [Lee13, Prop. 8.15]): first-order differential operators are characterized by being linear and satisfying the product rule.

Proposition 7.8. *If $L : C^\infty(\mathbb{R}^d) \to C^\infty(\mathbb{R}^d)$ is linear and satisfies the product rule, then there exist smooth coefficients $X^1, \dots, X^d$ so that*

$$(Lf)(x) = \sum_{i=1}^{d} X^i(x) \frac{\partial F}{\partial x^i}(x).$$

As a consequence, we see that any Poisson bracket must be given by a structure matrix $J : \mathbb{R}^d \to \mathbb{R}^{d\times d}$:

Corollary 7.9. *If $\{\cdot,\cdot\}$ is a Poisson bracket, then there exist smooth functions $J^{ij} : \mathbb{R}^d \to \mathbb{R}$ such that*

$$\{F, G\}(x) = \sum_{i,j=1}^{d} J^{ij}(x) \frac{\partial F}{\partial x^i} \frac{\partial G}{\partial x^j}.$$

Moreover, J is antisymmetric ($J^{ij} = -J^{ji}$ for all i, j) and we have the Jacobi identity:

$$\sum_{k=1}^{d} \left(\frac{\partial J^{ij}}{\partial x^k} J^{k\ell} + \frac{\partial J^{\ell i}}{\partial x^k} J^{kj} + \frac{\partial J^{j\ell}}{\partial x^k} J^{ki} \right) = 0 \tag{7.14}$$

for all i, j, ℓ. Lastly, $\{\cdot,\cdot\}$ is nondegenerate if and only if $\det J$ *is nonvanishing.*

Next, we turn to some examples. In the case $d = 2n$, our first definition (7.10) of the Poisson bracket provides a key example:

Example 7.10 (Canonical Poisson bracket)**.** Let (q, p) denote the coordinates on $\mathbb{R}^n \times \mathbb{R}^n$, and consider the canonical Poisson bracket (7.10). The structure matrix for this bracket in these coordinates is

$$J_0 = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

The properties of Definition 7.7 are easily verifiable for this matrix. Equivalently, the entries of this matrix are uniquely determined by the relations

$$\{q_i, q_j\} = 0 = \{p_i, p_j\}, \quad \{q_i, p_j\} = \delta_{ij} \quad \text{for all } i, j = 1, \dots, n.$$

These relations are called **Hamilton's commutation relations** or the **canonical relations**, and they are one of the remnants of quantum mechanics for macroscopic dynamics.

The matrix J_0 has the property that $J_0^2 = -I$. Consequently, we may think of J_0 as (a choice of) $\sqrt{-1}$, which is part of the reason why we use the letter

J. Indeed, nondegenerate Poisson brackets are closely related to "almost complex structures"; this relationship is further explored for the canonical structure matrix J_0 in Exercise 9.5.

We can also have a Poisson bracket on $\mathbb{R}^d$ for $d \neq 2n$:

Example 7.11 (Casimirs)**.** We augment Example 7.10 by adding coordinates y^i with

$$\{F, y^i\} \equiv 0$$

for all smooth F. Any such function y^i is called a **Casimir**. The structure matrix is now

$$J = \begin{pmatrix} 0 & I & 0 \\ -I & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

In canonical coordinates, introducing Casimirs is relatively uninteresting; however, the ability to identify a Casimir for an arbitrary Poisson bracket turns out to be quite useful in practice.

7.4. Hamiltonian vector fields

Given a first-order ODE

$$\dot{\mathbf{x}} = \mathbf{f}(t, \mathbf{x}),$$

we saw in (7.8) that the material derivative of an observable is $F(x)$ is the advection term $\mathbf{f} \cdot \nabla F$. Consequently, we can identify the RHS $\mathbf{f}$ geometrically with the vector field $\mathbf{f} \cdot \nabla$. As a choice of Poisson bracket and Hamiltonian produce a first-order ODE via (7.8), we would now like to explore this connection in terms of vector fields.

Specifically, the map $F \mapsto \{F, H\}$ defines a vector field X_H via

$$\{F, H\} = X_H(F), \quad \text{where} \quad X_H = J\nabla H, \quad X_H^i = \sum_{j=1}^{d} J^{ij}(x) \frac{\partial H}{\partial x^j}.$$

(Again, there is another popular convention that comes from swapping the order of F and H in the definition of $\{F, H\}$.) We call X_H the **Hamiltonian vector field** associated to H. This is not the only way that we can turn an observable H into a vector field. Indeed, the gradient vector field ∇H induces the gradient flow (cf. (2.5)), and this is associated to the dot product structure $F \mapsto \nabla F \cdot \nabla H$. The Hamiltonian vector field is the analogous object for the Poisson structure.

In Hamiltonian mechanics, the state of the system is described by a point x in $\mathbb{R}^d$ (or on a manifold) endowed with a Poisson structure. The evolution is dictated by a **Hamiltonian** (or **total energy**) $H : \mathbb{R}^d \to \mathbb{R}$ via **Hamilton's equations**

$$\dot{x} = X_H = J\nabla H. \tag{7.15}$$

Equivalently, the evolution of an observable $F(x)$ is

$$\dot{F} = \nabla F \cdot \dot{x} = \nabla F \cdot X_H = \sum_{i,j=1}^{d} J^{ij} \frac{\partial F}{\partial x^i} \frac{\partial H}{\partial x^j} = \{F, H\}.$$

These are the generalization of (7.2) and (7.11) to arbitrary Poisson structures. For future reference, we also note that the above calculation implies

$$X_H F = \{F, H\} = -\{H, F\} = -X_F H. \tag{7.16}$$

In other words, the evolution of F under the flow of H can be recast as the evolution of H under the flow of F.

Example 7.12. To put classical mechanics in this framework, we adopt the canonical bracket of Example 7.10. Here, q_i are the position coordinates and p_i are the corresponding momenta. The Hamiltonian is the total energy

$$H(q, p) = \tfrac{1}{2m^2} p^2 + V(q).$$

This yields the familiar equations of motion:

$$\begin{aligned} \dot{q} &= \{q, H\} = \tfrac{1}{2m} 2p\{q, p\} + V'(q)\{q, q\} = \tfrac{p}{m} + 0, \\ \dot{p} &= \{p, H\} = \tfrac{1}{2m} 2p\{p, p\} + V'(q)\{p, q\} = 0 - V'(q), \end{aligned}$$

where we used that the Poisson bracket satisfies the chain rule (7.12). The first equation is the definition of momentum, and the second equation is Newton's equation.

Example 7.13. For a free relativistic particle, the total energy is given by Einstein's equation

$$H = \sqrt{c^2 p^2 + m^2 c^4}.$$

This yields

$$\dot{q} = \frac{cp}{\sqrt{m^2 c^2 + p^2}}, \quad \dot{p} = 0.$$

In particular, we see that $|\dot{q}| \leq c$ with equality if and only if $m = 0$. These equations of motion can be used to derive the Lorentz formulas, which lie at the heart of relativistic mechanics. In fact, Hamiltonian mechanics is compatible with relativity. However, relativity is not built in to the Hamiltonian framework, and It turns out to be easier to incorporate relativity into Lagrangian mechanics.

Next, we record some easy consequences:

Lemma 7.14. *(a) The observable F is conserved under the flow of H if and only if $\{F, H\} \equiv 0$ (and we may swap F, H in either of these statements).*

(b) We have $[X_F, X_H] = -X_{\{F,H\}}$.

(c) If $\{F, H\}$ is a constant, then the F-flow commutes with the H-flow.

Proof. (a) This follows from the definition $X_H F = \{F, H\}$, and we may swap F and H in either statement by the observation (7.16).

(b) We compute

$$\begin{aligned} X_F(X_H G) &= X_F\{G, H\} = \{\{G, H\}, F\}, \\ X_H(X_F G) &= \{\{G, F\}, H\} = -\{\{F, G\}, H\}. \end{aligned}$$

Subtracting these and recalling the Jacobi identity, we have

$$\begin{aligned} [X_F, X_H]G &= \{\{G, H\}, F\} + \{\{F, G\}, H\} \\ &= -\{\{H, F\}, G\} = -\{G, \{F, H\}\} = -X_{\{F,H\}}G. \end{aligned}$$

(c) Note that $0 = [X_F, X_H] = -X_{\{F,H\}}$ requires that

$$\sum_{j=1}^{d} J^{ij} \frac{\partial}{\partial x^j}\{F, H\} = 0.$$

In particular, this happens if the gradient of $\{F, H\}$ vanishes. □

Example 7.15. Consider the canonical Poisson bracket on $\mathbb{R}^3$. The components of the angular momentum $\mathbf{L} = \mathbf{q} \times \mathbf{p}$ generate rotation about the corresponding coordinate axes. More generally, the flow of the Hamiltonian $\mathbf{a} \cdot \mathbf{L}$ is rotation about the $\mathbf{a}$-axis. Thus, if H is conserved by rotations, then part (a) allows us to turn this statement around: the flow of H conserves $\mathbf{L}$. Analogous conclusions hold for just component-wise conservation. Note how this is an example of Noether's theorem: a symmetry implies a conservation law.

To conclude this section, we will record one more observation about Poisson bracket:

Proposition 7.16 (Poisson's theorem)**.** *If the observables F and G are conserved under the flow of H, then their Poisson bracket $\{F, G\}$ is also conserved.*

Proof. We use the Jacobi identity (7.13) and note that $\{F, H\} = 0 = \{G, H\}$:

$$\begin{aligned} 0 &= \{\{F, G\}, H\} + \{\{G, H\}, F\} + \{\{H, F\}, G\} \\ &= \{\{F, G\}, H\} + \{\{G, H\}, F\} - \{\{F, H\}, G\} \\ &= \{\{F, G\}, H\}. \end{aligned}$$

The RHS is exactly the time derivative of $\{F, G\}$ under the flow of H. □

Example 7.17. If $L_1 = x_2p_3 - x_3p_2$ and $L_2 = x_3p_1 - x_1p_3$ are the first and second components of the angular momentum $\mathbf{L} = \mathbf{x} \times \mathbf{p}$ of a particle $\mathbf{x} \in \mathbb{R}^3$, then their bracket

$$\{L_1, L_2\} = \{x_2p_3, x_3p_1\} + \{x_3p_2, x_1p_3\} = -x_2p_1 + p_2x_1 = L_3$$

is the remaining component of the angular momentum.

Although powerful, it should be noted that the new quantity $\{F, G\}$ is not guaranteed to be nontrivial. For example, a system with n degrees of freedom can only have up to $2n - 1$ independent conserved quantities, and so repeated applications of Proposition 7.16 must eventually stop producing independent quantities.

7.5. Darboux theorem

Now that we have a general notion of a Poisson structure on $\mathbb{R}^d$, we would like to understand what the possibilities are for how it behaves locally. The Darboux theorem says that Example 7.11 is in fact the only possibility. Although this result most commonly is associated with Darboux, the Poisson bracket formulation is due to Lie [Lie80].

Theorem 7.18 (Darboux theorem)**.** *If the rank of $J(x)$ is independent of x, then for any $x_0 \in \mathbb{R}^d$ there exist coordinates $(p_1, \dots, p_n, q_1, \dots, q_n, y_1, \dots, y_k)$ on a neighborhood of x_0 so that*

$$\{q_j, p_j\} = \delta_{ij}, \quad \{p_i, p_j\} = 0 = \{q_i, q_j\}, \quad \{\cdot, y_\ell\} = 0$$

for all i, j, ℓ.

If the rank of $J(x)$ is full—i.e. the Poisson bracket is nondegenerate—then this immediately implies the well-known Darboux theorem about symplectic structures (Theorem 9.3).

If the rank of $J(x)$ is not full, then we must have $k \geq 1$ many coordinates y_ℓ. Such an observable y_ℓ is called a **Casimir**. Note that $\{\cdot, y_\ell\} = 0$ implies that y_ℓ is conserved by all Hamiltonian flows.

Proof. We follow the proof from [Wei83].

Fix $x_0 \in \mathbb{R}^d$. For ease of notation, we translate so that $x_0 = 0$. We will induct on the rank of J near x_0.

For the base case, suppose that the rank of J is zero near x_0. Then $J \equiv 0$, and so we take $y_1, \dots, y_d$ to be any coordinates on $\mathbb{R}^d$.

Next we turn to the inductive step. Assume that the rank of J near x_0 is nonzero. Choose a function p_1 so that $X_{p_1}(x_0) \neq 0$. In particular, we must have $\nabla p_1(x_0) \neq 0$. By Proposition A.18, we can pick a full set of coordinates $x_1, \dots, x_d$ so that $\frac{\partial}{\partial x_1} = X_{p_1}$. We then take $q_1(x) = x_1$, which automatically satisfies

$$\{q_1, p_1\} = X_{p_1} q_1 = \frac{\partial}{\partial x_1} x_1 = 1.$$

We claim that X_{p_1} and X_{q_1} at x_0 must be linearly independent. Suppose that $\lambda X_{p_1} + \mu X_{q_1} = 0$ at x_0 for some $\mu, \lambda \in \mathbb{R}$. Then

$$\begin{aligned}(\lambda X_{p_1} + \mu X_{q_1}) q_1 &= \lambda \{q_1, p_1\} + \mu \{q_1, q_1\} = \lambda, \\ (\lambda X_{p_1} + \mu X_{q_1}) p_1 &= -\mu,\end{aligned}$$

and so $\lambda = \mu = 0$ as desired.

By the claim and Proposition A.19, we can find a new full set of coordinates $x_1, \dots, x_d$ so that

$$\frac{\partial}{\partial x_1} = X_{p_1}, \quad \frac{\partial}{\partial x_2} = X_{q_1}.$$

It is important to know that it is possible to extend to a full set of coordinates at this step. Indeed, in order to even define $\frac{\partial}{\partial x_1}$ we need a full set of coordinates. (In statistical mechanics, the notation $(\frac{\partial E}{\partial V})_P$ is expressly intended to resolve this issue.)

Next we claim that $(p_1, q_1, x_3, \dots, x_d)$ are also valid coordinates on a neighborhood of x_0—i.e. their gradients at x_0 are linearly independent. Suppose that

$$0 = \nabla\left(c_1 p_1 + c_2 q_2 + \sum_{\ell=3}^{d} c_\ell x_\ell\right)(x_0)$$

for some constants $c_1, \dots, c_d$. Then

$$0 = \left\{c_1 p_1 + c_2 q_2 + \sum_{\ell=3}^{d} c_\ell x_\ell, p_1\right\} = c_1\{p_1, p_1\} + c_2\{q_1, p_1\} - \sum_{\ell=3}^{d} \frac{\partial x_\ell}{\partial x_1} = c_2,$$

and so $c_2 = 0$. Similarly,

$$0 = \left\{c_1 p_1 + c_2 q_2 + \sum_{\ell=3}^{d} c_\ell x_\ell, q_1\right\} = -c_1.$$

Now we have a linear combination of the gradients of $x_3, \dots, x_d$ at x_0, and since $x_1, \dots, x_d$ are coordinates then we must have $c_3 = \cdots = c_d = 0$ as desired.

Finally, we would like to invoke the inductive hypothesis for the Poisson structure restricted to the domain of $x_3, \dots, x_d$. First we check that $\{x_k, x_\ell\}$ are independent of p_1, q_1 for all $k, \ell = 3, \dots, d$. Using the Jacobi identity, we compute

$$\begin{aligned}\frac{\partial}{\partial x_1}\{x_k, x_\ell\} &= X_{p_1}\{x_k, x_\ell\} = \{\{x_k, x_\ell\}, p_1\} \\ &= -\{\{p_1, x_k\}, x_\ell\} - \{\{x_\ell, p_1\}, x_k\} = 0,\end{aligned}$$

where in the last equality we noted that the inner Poisson brackets vanish since $X_{p_1} = \partial_{x_1}$. A similar computation shows that

$$\frac{\partial}{\partial x_2}\{x_k, x_\ell\} = 0.$$

Therefore the Poisson bracket restricted to the domain of $x_3, \dots, x_d$ is well-defined and has its rank reduced by two. Indeed, by our construction the structure matrix J in the coordinates $x_1, \dots, x_d$ is a diagonal 2×2 block matrix with the 2×2 leading entry

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

By the inductive hypothesis, we can find a diffeomorphic change of variables from $(x_3, \dots, x_d)$ to $(q_2, \dots, q_n, p_2, \dots, p_n, y_1, \dots, y_k)$ near x_0 so that the new coordinates obey the canonical Poisson bracket relations. Adding in p_1, q_1 then yields the desired coordinates. □

7.6. Canonical transformations

A fundamental feature of the Hamiltonian perspective is that the positions and momenta are treated as independent coordinates. Physically, we know that this is not true—the momentum is defined in terms of the position by (1.1). Consequently, an arbitrary change of variables will not preserve the physical system. Canonical transformations are those changes of variables which are admissible.

Given a Poisson structure on $\mathbb{R}^d$, we call a map $\Psi : \mathbb{R}^d \to \mathbb{R}^d$ is **canonical** if it preserves the bracket:

$$\{F \circ \Psi, G \circ \Psi\} = \{F, G\} \circ \Psi \quad \text{for all } F, G. \tag{7.17}$$

In other words, Ψ satisfies

$$\sum_{i,j=1}^{d} \frac{\partial \Psi^k}{\partial x^i} J^{ij} \frac{\partial \Psi^\ell}{\partial x^j} = J^{k,\ell} \circ \Psi. \tag{7.18}$$

If J is also nondegenerate, then we call Ψ a **symplectomorphism** because the Poisson bracket induces a symplectic structure. Note that if Ψ is a symplectomorphism, then Ψ is automatically a diffeomorphism. Indeed, we can see that Ψ' is invertible by taking determinants in (7.18).

As a warning, some authors define canonical transformations as any diffeomorphism which preserves Hamilton's equations (7.2). It is false that these two definitions are equivalent, and this point is even neglected in the literature (cf. [LL76, Sec. 45]). Indeed, the condition that a transformation preserves Hamilton's equations (7.2) is weaker and less geometrically significant. For example $P = 2p$, $Q = q$ satisfies (7.2) but not (7.18).

The definition (7.18) is closely related to the **symplectic group** $\mathrm{Sp}(\mathbb{R}^{2n})$, which is comprised of the invertible $2n \times 2n$ matrices U such that

$$U^T J_0 U = J_0, \quad \text{where } J_0 = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \tag{7.19}$$

We will soon make this relationship precise in Proposition 7.20. Note that if we replace the canonical structure matrix J_0 by the identity matrix I then we recover the orthogonal group; this reflects that I is the structure matrix for the dot product.

First, we record some facts about $\mathrm{Sp}(\mathbb{R}^{2n})$:

Proposition 7.19. $\mathrm{Sp}(\mathbb{R}^{2n})$ *is a group that is closed under transposition.*

Proof. To see that $\mathrm{Sp}(\mathbb{R}^{2n})$ is a group, we check that it is closed under inversion. Suppose that U satisfies (7.19). Then U has nonzero determinant, and so by multiplying by U^{-1} and U^{-T} we see that $J_0 = U^{-T} J_0 U^{-1}$.

The group $\mathrm{Sp}(\mathbb{R}^{2n})$ is also closed under transposition. This does not follow from taking the transpose of (7.19) however, because taking the transpose of (7.19) does not yield anything new. Instead, we take the inverse of (7.19) to obtain $-U^{-1} J_0 U^{-T} = -J_0$. As $\mathrm{Sp}(\mathbb{R}^{2n})$ is closed under inversion, we conclude that $U^T \in \mathrm{Sp}(\mathbb{R}^{2n})$. □

In the case of the canonical Poisson bracket, we have:

Proposition 7.20. *Suppose $J = J_0$. Then Ψ is canonical if and only if $\Psi' \in \mathrm{Sp}(\mathbb{R}^{2n})$.*

Proof. The relation (7.18) reads $\Psi' J_0 (\Psi')^T = J_0$, and we know that $\mathrm{Sp}(\mathbb{R}^{2n})$ is closed under transposition. □

Note that the block matrix

$$U = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

lies in $\mathrm{Sp}(\mathbb{R}^{2n})$ if and only if

$$A^T C = C^T A, \quad B^T D = D^T B, \quad A^T D - C^T B = I. \tag{7.20}$$

Taking determinants, we see that $(\det U)^2 = 1$. It is not obvious, but we actually have $\det U = 1$; this is proved in Exercise 7.6. In particular, symplectic matrices preserve both volume and orientation.

The symplectic group is not only similar to the orthogonal group on $\mathbb{R}^{2n}$ and the unitary group on $\mathbb{C}^n$, but they are also deeply connected. One facet of this relationship is illustrated in Exercise 7.6. As a warning, unlike orthogonal and unitary matrices, symplectic matrix are not always diagonalizable. Indeed, from the conditions (7.20) we see that

$$\begin{pmatrix} I & B \\ 0 & I \end{pmatrix} \quad \text{with } B = B^T$$

is symplectic. When $B = I$, this matrix is essentially a Jordan block and hence is not diagonalizable.

Lastly, we record the following criteria to check if a transformation is canonical in practice:

Proposition 7.21. *Suppose that we have a nondegenerate Poisson structure on $\mathbb{R}^{2n}$. Then $\Psi(q,p) = (Q,P)$ is a canonical transformation (and hence a symplectomorphism) if and only if the new variables satisfy the canonical relations with respect to the old variables:*

$$\{Q_i, Q_j\}_{p,q} = 0, \qquad \{P_i, P_j\}_{p,q} = 0, \qquad \{P_i, Q_j\}_{p,q} = \delta_{ij}$$

for all $i, j = 1, \ldots, n$.

Proof. We may assume that the Poisson bracket is given in canonical coordinates (q, p) by Theorem 7.18.

The forward implication is immediate, since we can replace the differentiation variables q, p with Q, P by assumption. For example,

$$\{Q_i, Q_j\}_{q,p} = \{Q_i, Q_j\}_{Q,P} = 0.$$

For the reverse implication, the premise tells us that

$$\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} = \begin{pmatrix} \frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} \\ \frac{\partial P}{\partial q} & \frac{\partial P}{\partial p} \end{pmatrix} \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial Q}{\partial q} & \frac{\partial P}{\partial q} \\ \frac{\partial Q}{\partial p} & \frac{\partial P}{\partial p} \end{pmatrix}.$$

So given arbitrary observables F, G we have

$$\begin{aligned} \{F, G\}_{Q,P} &= \begin{pmatrix} \frac{\partial F}{\partial Q} & \frac{\partial F}{\partial P} \end{pmatrix} \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial G}{\partial Q} \\ \frac{\partial G}{\partial P} \end{pmatrix} \\ &= \begin{pmatrix} \frac{\partial F}{\partial Q} & \frac{\partial F}{\partial P} \end{pmatrix} \begin{pmatrix} \frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} \\ \frac{\partial P}{\partial q} & \frac{\partial P}{\partial p} \end{pmatrix} \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial Q}{\partial q} & \frac{\partial P}{\partial q} \\ \frac{\partial Q}{\partial p} & \frac{\partial P}{\partial p} \end{pmatrix} \begin{pmatrix} \frac{\partial G}{\partial Q} \\ \frac{\partial G}{\partial P} \end{pmatrix} \\ &= \begin{pmatrix} \frac{\partial F}{\partial q} & \frac{\partial F}{\partial p} \end{pmatrix} \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial G}{\partial q} \\ \frac{\partial G}{\partial p} \end{pmatrix} = \{F, G\}_{q,p}. \end{aligned}$$

Therefore Ψ preserves the Poisson bracket in the sense of (7.17). □

7.7. Liouville's theorem

In this section we will prove Liouville's theorem, which says that Hamiltonian flows preserve Lebesgue measure on phase space. In other words, the density of trajectories in phase space surrounding a given trajectory is constant in time.

Given a Borel measure μ on $\mathbb{R}^d$, we say that a continuous map $\Phi : \mathbb{R}^d \to \mathbb{R}^d$ **preserves the measure** μ if

$$\mu(\Phi^{-1}(A)) = \mu(A) \quad \text{for all } A \subset \mathbb{R}^d \text{ Borel measurable.} \tag{7.21}$$

(As in measure theory, we need to use Φ^{-1} here instead of Φ because $\Phi^{-1}(A)$ is Borel when A is by the continuity of Φ, but $\Phi(A)$ might not be.) The condition (7.21) is equivalent to

$$\int (f \circ \Phi)(x) \, \mathrm{d}\mu(x) = \int f(x) \, \mathrm{d}\mu(x) \quad \text{for all } f \in C_c^\infty(\mathbb{R}^d). \tag{7.22}$$

Indeed, note that taking $f = 1_A$ in (7.22) yields (7.21), and the equivalence is proved by approximating 1_A by smooth functions. The equations (7.21)-(7.22) is also sometimes conveyed by saying that the pushforward measure $\mu \circ \Phi^{-1}$ is equal to μ. (Recall that measures pushforward because they are dual to functions, which pullback.)

Liouville's theorem follows from the following general fact about ODEs:

Lemma 7.22. *Let X be a smooth autonomous vector field on $\mathbb{R}^d$ and $\omega \in C^\infty(\mathbb{R}^d)$. Then the flow of $\dot{\mathbf{x}} = X(\mathbf{x})$ preserves the measure $\omega(x)\,dx$ if and only if $\nabla \cdot (\omega X) \equiv 0$.*

Proof. Let $\Phi(t;\boldsymbol{\xi})$ denote the solution $\mathbf{x}(t;\boldsymbol{\xi})$ to the differential equation $\dot{\mathbf{x}} = X(\mathbf{x})$ with initial data $\mathbf{x}(0) = \boldsymbol{\xi}$.

For the forward direction, assume that the flow preserves $\omega(x)\,\mathrm{d}x$. For a smooth compactly supported observable $F(t,\mathbf{x})$ we take the pullback by Φ:

$$\begin{aligned}\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \int (F\circ\Phi)(t,\boldsymbol{\xi})\omega(\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi} &= \int X(\boldsymbol{\xi})\cdot\nabla F(\boldsymbol{\xi})\omega(\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi} \\ &= -\int F(\boldsymbol{\xi})\nabla\cdot(\omega X)(\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi}.\end{aligned}$$

By premise, the LHS vanishes. As $F \in C_c^\infty$ was arbitrary, we conclude that $\nabla\cdot(\omega X) \equiv 0$ as desired.

For the reverse direction, assume that $\nabla\cdot(\omega X) \equiv 0$. Using $\dot{\Phi} = X\circ\Phi$ and the derivative (A.15) of the determinant, we compute

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}(\omega\circ\Phi)(t,\boldsymbol{\xi})\det D_{\boldsymbol{\xi}}\Phi(t,\boldsymbol{\xi}) \\ &= \left\{(\nabla\omega\circ\Phi)(t,\boldsymbol{\xi})\cdot(X\circ\Phi)(t,\boldsymbol{\xi}) + \left(\omega\cdot\sum_{i=1}^d \frac{\partial X_i}{\partial \boldsymbol{\xi}_i}\right)\circ\Phi(t,\boldsymbol{\xi})\right\}\det D_{\boldsymbol{\xi}}\Phi(t,\boldsymbol{\xi}) \\ &= \big[\nabla\cdot(\omega X)\big]\circ\Phi(t,x)\det D_{\boldsymbol{\xi}}\Phi(t,\boldsymbol{\xi}).\end{aligned}$$

The RHS vanishes by premise, and so we conclude that the quantity in the time derivative on the LHS is equal to its initial value:

$$\omega\circ\Phi(t,\boldsymbol{\xi})\det D_{\boldsymbol{\xi}}\Phi(t,\boldsymbol{\xi}) = \omega(\boldsymbol{\xi})\det I = \omega(\boldsymbol{\xi}) \quad \text{for all } t.$$

Consequently, the change of variables $x = \Phi(t,\boldsymbol{\xi})$ yields

$$\begin{aligned}\int (F\circ\Phi)(t,\boldsymbol{\xi})\omega(\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi} &= \int (F\circ\Phi)(t,\boldsymbol{\xi})(\omega\circ\Phi)(t,\boldsymbol{\xi})\det D_{\boldsymbol{\xi}}\Phi(t,\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi} \\ &= \int F(\boldsymbol{\xi})\omega(\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi}.\end{aligned}$$

This is exactly the condition (7.22), and so we conclude that the flow Φ preserves $\omega(x)\,\mathrm{d}x$. □

As an immediate corollary, we obtain Liouville's theorem for the canonical Poisson bracket:

Proposition 7.23 (Liouville's theorem, special case)**.** *Suppose that $J = J_0$ is the canonical Poisson bracket. Then any Hamiltonian flow on $\mathbb{R}^{2n}$ preserves the Lebesgue measure.*

Proof. Given a Hamiltonian H, the corresponding Hamiltonian vector field is

$$X_H = \left(\frac{\partial H}{\partial p}, -\frac{\partial H}{\partial q} \right).$$

This vector field is divergence-free since

$$\nabla \cdot X_H = \frac{\partial^2 H}{\partial q \partial p} - \frac{\partial^2 H}{\partial p \partial q} \equiv 0,$$

and so its flow preserves Lebesgue measure by Lemma 7.22. □

Next, we would like to extend this fact to all Poisson structures. First, we will need:

Proposition 7.24. *The flow map $\Phi(t, \cdot)$ of any Hamiltonian vector field is canonical.*

Proof. By Theorem 7.18, we may work in local coordinates so that

$$J = \begin{pmatrix} 0 & I & 0 \\ -I & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

is independent of x. Given a Hamiltonian H, the flow map $\Phi(t, x)$ is defined by

$$\frac{\partial \Phi}{\partial t} = J(\nabla H) \circ \Phi,$$

and so

$$\frac{\partial \Phi'}{\partial t} = J(H'' \circ \Phi)\Phi'.$$

Let

$$E(t) = \Phi' J (\Phi')^T - J$$

denote the failure of Φ to be symplectic. Then

$$\begin{aligned} \frac{\mathrm{d}E}{\mathrm{d}t} &= J(H'' \circ \Phi)\Phi' J(\Phi')^T + \Phi' J(\Phi')^T (H'' \circ \Phi)^T J^T \\ &= J(H'' \circ \Phi)(E + J) - (E + J)(H'' \circ \Phi)^T J^T \\ &= J(H'' \circ \Phi)E - E(H'' \circ \Phi)J, \end{aligned}$$

where in the second equality we noted that H'' is symmetric and J is antisymmetric. The RHS is a bounded linear operator applied to E, and so we conclude that there exists a constant C so that

$$\left| \frac{\mathrm{d}E}{\mathrm{d}t}(t) \right| \leq C|E(t)|.$$

As $E(0) = 0$, then Grönwall's inequality (Lemma A.3) implies $E(t) \equiv 0$ as desired. □

We are now prepared to prove:

Theorem 7.25 (Liouville's theorem, general case)**.** *For a nondegenerate Poisson structure J, any canonical mapping Φ preserves* ***phase volume****:*

$$\int (f \circ \Phi)(x) |\det J(x)|^{-\frac{1}{2}}\, dx = \int f(y) |\det J(y)|^{-\frac{1}{2}}\, dy \quad \text{for all } f \in C_c^\infty(\mathbb{R}^d).$$

In particular, this holds for the flow map of any Hamiltonian vector field.

Proof. Consider the change of variables

$$y = \Phi(x), \quad \mathrm{d}y = |\det \Phi'|\, \mathrm{d}x.$$

As $J \circ \Phi = \Phi' J (\Phi')^T$, we have

$$\int f(y) \frac{\mathrm{d}y}{|\det J(y)|^{\frac{1}{2}}} = \int (f \circ \Phi)(x) \frac{|\det \Phi'|\, \mathrm{d}x}{|\det J \circ \Phi|^{\frac{1}{2}}} = \int (f \circ \Phi)(x) \frac{\mathrm{d}x}{|\det J|^{\frac{1}{2}}}. \quad \square$$

Liouville's theorem has many important consequences. For example, we now know that for a Hamiltonian system there can be no asymptotically stable equilibrium points or asymptotically stable closed trajectories in phase space, since these would require that the density of phase curves to increase around such phenomena. We also have the following phenomenon:

Corollary 7.26 (Poincare's recurrence theorem)**.** *Fix $t \in \mathbb{R}$ and $D \subset \mathbb{R}^{2n}$ a bounded region of phase space, and let $\Phi := \Phi(t, \cdot)$ denote the flow by time t of a Hamiltonian vector field. Then for any positive measure set $U \subset D$ there exists $x_0 \in U$ and a positive integer n such that $\phi^n(x_0) \in U$.*

If the motion is bounded—as is the case for a conservative Newtonian system with potential energy $V(\mathbf{x}) \to +\infty$ as $|\mathbf{x}| \to \infty$—this means that the system will return to an arbitrary vicinity of any given possible configuration $(q, p) \in \mathbb{R}^{2d}$ infinitely often, given enough time. For example, suppose we opened a connection between chambers of gas and vacuum. Then Corollary 7.26 says that the gas molecules will eventually all return to the initial chamber, seemingly in violation of the second law of thermodynamics. Although it may appear that Poincare's theorem conflicts with Liouville's theorem, the time scales are often quite large (in our example it is longer than the age of the universe) and so there is no contradiction.

Proof. Given a smooth Hamiltonian, Hamilton's equations are a smooth system of ODEs and so the subsequent flow $\Phi : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is injective by uniqueness of solutions. Liouville's theorem (Theorem 7.25) tells us that Φ preserves phase volume.

Consider the collection of sets $U, \Phi(U), \Phi^2(U), \cdots \subset D$. As Φ is volume-preserving, all of these sets must have the same volume. On the other hand, D is bounded and thus has finite volume, and so it is impossible for all of these sets to be disjoint. That is, there exists some distinct $j < k$ such that $\Phi^j(U) \cap \Phi^k(U) \neq \emptyset$. As Φ is injective, this requires $\Phi^{k-j}(U) \cap U \neq \emptyset$. Namely, we can pick some $x_0 \in U$ in this intersection, which gives $\phi^{k-j}(x_0) \in U$. $\square$

In fact, the proof of Corollary 7.26 shows that the set of points in U which do not return to U infinitely often has measure zero.

Together, a measure space X with a finite measure μ and a measurable function $\phi : X \to X$ that is measure preserving constitute a measure preserving space, which is the fundamental object of study in discrete dynamical systems.

In fact, phase volume is the only measure on phase space that can be preserved:

Proposition 7.27. *Suppose that J is nondegenerate. If a smooth measure $\omega(x)\,dx$ is invariant under all Hamiltonian flows, then it must be a scalar multiple of the phase volume measure.*

Proof. By Theorem 7.18, we may work in local canonical coordinates. Suppose that he measure

$$\omega(p_1, \dots, p_n, q_1, \dots, q_n)\,\mathrm{d}p_1 \dots \mathrm{d}p_n\,\mathrm{d}q_1 \dots \mathrm{d}q_n$$

is invariant under all Hamiltonian flows. Taking the Hamiltonian $H = p_k$ we have the vector field $X_H = \frac{\partial}{\partial q_k}$, and so Lemma 7.22 requires that

$$0 = \nabla \cdot (\omega X_H) = \frac{\partial \omega}{\partial q_k}$$

for all k. Taking $H = q_k$, we similarly conclude that $\frac{\partial \omega}{\partial p_k} = 0$ for all k. Therefore $\nabla \omega \equiv 0$, and hence ω is a constant. □

Let

$$\mathrm{d}\nu := |\det J(x)|^{-\frac{1}{2}}\,\mathrm{d}x$$

denote the phase volume measure. The **Gibbs' measure** or **Gibbs' state** associated to a Hamiltonian system at temperature $T > 0$ is

$$\tfrac{1}{Z} e^{-\beta H}\,\mathrm{d}\nu,$$

where $\beta = \frac{1}{k_B T}$, Boltzman's constant k_B is a universal constant, and the partition function Z is a normalization constant chosen so that the total integral of the Gibbs' measure is one. Note that this definition requires that $e^{-\beta H}$ is integrable. When the temperature T is small, β is large and hence the Gibbs' measure is supported near the minima of H. When T is large, β is small and the Gibb's measure is supported more evenly everywhere.

The Gibbs' measure can also be characterized via a variational principle, but this still requires phase volume (via the entropy). On the other hand, we also have the following algebraic characterization:

Proposition 7.28. *The Gibbs' state is the unique probability measure that satisfies the **classical Kubo–Martin–Swinger** (KMS) **condition**:*

$$\mathbb{E}[\{F, G\}] = \beta \mathbb{E}[\{F, H\}G] \quad \textit{for all } F, G \in C_c^\infty(\mathbb{R}^d).$$

Here, the expected value $\mathbb{E}$ is defined in terms of a probability measure $\omega(x)\,dx$ via

$$\mathbb{E}[X] = \int X(x)\omega(x)\,dx.$$

Proof. The KMS condition says that

$$\begin{aligned}\mathbb{E}[e^{\beta H}\{F, Ge^{-\beta H}\}] &= \mathbb{E}[e^{\beta H}(\{F,G\}e^{-\beta H} - \beta e^{-\beta H}\{F,H\}G)] \\ &= \mathbb{E}[\{F,G\}] - \beta\mathbb{E}[\{F,H\}G] = 0.\end{aligned}$$

So if a probability measure $\omega(x)\,\mathrm{d}x$ satisfies the KMS condition, then

$$\mathbb{E}[e^{\beta H}\{F,K\}] = 0 \quad \text{for all } F, K \in C_c^\infty(\mathbb{R}^d).$$

In other words,

$$\int (\omega e^{\beta H})\{F,K\}\,\mathrm{d}x \quad \text{for all } F, K \in C_c^\infty(\mathbb{R}^d).$$

Therefore $\omega e^{\beta H}\,\mathrm{d}x$ is a measure that is invariant under all Hamiltonian flows, and hence $\omega e^{\beta H}\,\mathrm{d}x$ is proportional to the phase volume $\mathrm{d}\nu$. Rearranging, we see that ω is equal to the Gibbs' measure as claimed. □

Example 7.29. Consider an infinite chain of oscillators, with Hamiltonian

$$H = \sum_{i\in\mathbb{Z}} [\tfrac{1}{2}p_i^2 + V(q_i - q_{i-1})].$$

Well-posedness for such an infinite-dimensional system is not an issue (cf. Theorem A.2) and neither is defining a measure on this infinite-dimensional space (cf. sequences of random variables in probability theory). However, $H = +\infty$ almost everywhere, and so the factor $e^{-\beta H} \equiv 0$ in the Gibbs' measure does not make sense. Nevertheless, the KMS condition does make sense, if we also require that F, G depend on finitely many variables. Using this, we could proceed to define a Gibbs' measure.

7.8. Exercises

7.1 (Charged particle in an electromagnetic field)**.** In Exercise 4.7, we found the Lagrangian for a charged particle in $\mathbb{R}^3$ with charge q and mass m moving through an electromagnetic field to be

$$\mathscr{L} = \tfrac{1}{2}mv^2 - q\phi + \tfrac{q}{c}v \cdot A$$

where ϕ and A are the scalar and vector potentials for the electric and magnetic fields:

$$B = \nabla \times A, \qquad E = -\nabla\phi - \frac{1}{c}\frac{\partial A}{\partial t}.$$

(a) Show that the Hamiltonian for this system is

$$H = \tfrac{1}{2m}\left(p - \tfrac{q}{c}A\right)^2 + q\phi.$$

(b) Although the electric and magnetic fields are uniquely expressed, the scalar and vector potentials that ϕ and A are not unique and they appear explicitly in the Hamiltonian. In fact, substituting $A' = A + \nabla f$ for any smooth function $f(t, \mathbf{x})$ leaves B unchanged since the curl of a gradient is also zero. Show that for E to remain unchanged we need to also substitute

$$\phi' = \phi - \frac{1}{c}\frac{\partial f}{\partial t}.$$

Together, replacing $(A, \phi) \to (A', \phi')$ is called a **gauge transformation**, and a specific pair (A, ϕ) is called a choice of **gauge**.

(c) As the electric and magnetic fields are unaffected by the choice of gauge, then any physical laws in terms of the potentials should also be invariant. Show that under a gauge transformation the Hamiltonian becomes

$$H' = H - \frac{q}{c}\frac{\partial f}{\partial t},$$

and that Hamilton's equations still hold in the new variables.

7.2 (Young's inequality)**.** Show that for any Legendre transform pair $f(\mathbf{x})$ and $f^*(\boldsymbol{\xi})$ we have

$$\mathbf{x} \cdot \boldsymbol{\xi} \leq f(\mathbf{x}) + f^*(\boldsymbol{\xi}) \quad \text{for all } \mathbf{x}, \boldsymbol{\xi} \in \mathbb{R}^n.$$

Apply this inequality to the function $f(\mathbf{x}) = |\mathbf{x}|^p/p$ for $p \in (1, \infty)$ and conclude

$$\mathbf{x} \cdot \boldsymbol{\xi} \leq \frac{|\mathbf{x}|^p}{p} + \frac{|\boldsymbol{\xi}|^q}{q}, \quad \text{where } \tfrac{1}{p} + \tfrac{1}{q} = 1.$$

7.3 (Properties of the Legendre transform)**.** Suppose that $f : \mathbb{R}^n \to (-\infty, +\infty]$ is lower semicontinuous and not identically $+\infty$.

(a) Define the sub-differential

$$\partial f(\mathbf{x}) = \{\mathbf{v} \in \mathbb{R}^n : f(\mathbf{y}) - f(\mathbf{x}) \geq \mathbf{v} \cdot (\mathbf{y} - \mathbf{x}) \text{ for all } \mathbf{y} \in \mathbb{R}^n\}.$$

Show that if f is convex, then $\partial f(\mathbf{x})$ is nonempty for all $\mathbf{x} \in \mathbb{R}^n$. Show that the Legendre transform $f^*(\boldsymbol{\xi})$ (defined by (7.5)) is equal to $\mathbf{x}\cdot\boldsymbol{\xi} - f(\mathbf{x})$ if and only if $\boldsymbol{\xi} \in \partial f(\mathbf{x})$.

(b) Show that $f^*(\boldsymbol{\xi})$ is a lower semicontinuous and convex function. Moreover, show that f^{**} is the largest lower semicontinuous convex function that is less than or equal to f, and $f^{**} = f$ if f is convex.

7.4 (Example of Poisson's theorem)**.** Let $\mathbf{L} = \mathbf{x} \times \mathbf{p}$ denote the angular momentum of a particle $\mathbf{x} \in \mathbb{R}^3$. Show that for any unit vector $\mathbf{n}$ we have

$$\{\mathbf{L}, \mathbf{L} \cdot \mathbf{n}\} = \mathbf{L} \times \mathbf{n}.$$

(Hint: Fix Cartesian coordinates with respect to $\mathbf{n}$ and write down the vector field corresponding to rotation about the $\mathbf{n}$ axis. Apply this vector field to $\mathbf{L}$ and recognize this as the canonical Poisson bracket of $\mathbf{L}$ with a certain Hamiltonian. Conclude that $\{L_i, L_j\} = -L_k$ whenever i, j, k is a cyclic permutation of $1, 2, 3$.)

7.5 (Chain rule for Poisson brackets)**.** Given a Poisson bracket in the sense of Definition 7.7, show that we have the chain rule

$$\{V(q), F\} = V'(q)\{q, F\}.$$

(Hint: Use the product rule of Definition 7.7 and the Taylor expansion $V(q) = V(q_0) + V'(q_0)(q - q_0) + (q - q_0)^2 W(q)$.)

7.6. (a) Show that a symplectic matrix M is orthogonal if and only if it takes the form

$$\begin{bmatrix} A & B \\ -B & A \end{bmatrix}$$

with matrices A and B such that $A + iB$ is a complex unitary matrix. (Hint: For the reverse direction, start with the relation $M^T(I + iJ)M = I + iJ$.)

(b) Deduce that such matrices have determinant equal to 1. (Hint: Use a complex matrix to diagonalize M.)

7.7. Hamilton's equations also arise from a variational principle, but the functional is unbounded and hence less useful. Given a smooth and strictly convex Hamiltonian $H : \mathbb{R}^{2n} \to \mathbb{R}$ with $H(0) = 0$ and an energy level $\alpha \in \mathbb{R}$, consider the functional

$$E(\mathbf{x}(t)) = \tfrac{1}{2} \int_0^1 \mathbf{x}(t) \cdot J\dot{\mathbf{x}}(t)\, \mathrm{d}t$$

with the domain

$$M_\alpha = \left\{ \mathbf{x} \in C^1(\mathbb{R}; \mathbb{R}^{2n}) : \mathbf{x}(t+1) = \mathbf{x}(t),\ \int_0^1 H(\mathbf{x}(t))\, \mathrm{d}t = \alpha \right\}.$$

Here, J is the canonical structure matrix (9.6). Show that if $\mathbf{x}(t)$ is a critical point of E on M_α, then $\mathbf{x}(t) = (\mathbf{q}(t), \mathbf{p}(t))$ is a periodic solution of Hamilton's equations (7.2). Show that E is not bounded below on $\{x \in C^1(\mathbb{R}; \mathbb{R}^{2n}) : \mathbf{x}(t+1) = \mathbf{x}(t)\}$.

CHAPTER 8

NORMAL FORMS

We will study the local structure of Hamiltonian flows in a neighborhood of a point, with a focus on common physical examples. The material for this chapter is based upon various sections from [Arn89, MZ05].

8.1. Generating functions

In practice, we would like a way of coming up with transformations $\Phi : (q, p) \mapsto (Q, P)$ that are canonical as defined in (7.17). In Proposition 7.24 we saw that one way to do this is to use the flow of a Hamiltonian by some fixed time. In this section we will present another method: generating functions. In fact, this will provide a characterization of canonical transformations that are close to the identity in a certain sense. We will also refer to this material in section 8.4.

As we will see shortly, canonical transformations $\Phi(q, p) = (Q, P)$ near the identity are determined by a function W of the *initial* position q and the *final* momentum P. Specifically, $W(q, P)$ is the **generating function** of the transformation Φ if

$$p = \frac{\partial W}{\partial q}, \qquad Q = \frac{\partial W}{\partial P}.$$

For example,

$$W = Pq$$

is the generating function for the identity map. Although it may be surprising at first, it is crucial that the function W depends on some of the the initial and finial variables. On the other hand, we have some choice as to which variables we pick for W to depend on. Indeed, we can do something similar with generating functions of q, Q, but this does not encode the identity transformation (and thus it corresponds to canonical transformations that are far from the identity).

These generating functions $W(q, P)$ characterize canonical transformations in the following sense:

Theorem 8.1. *Consider $\mathbb{R}^{2n}$ endowed with the canonical Poisson bracket $J = J_0$ and a function $\Phi : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ and write $\Phi(p, q) = (P(p, q), Q(p, q))$.*

(a) *If Φ is canonical and* $\det \frac{\partial P}{\partial p} \neq 0$*, then there exists a function $W(q,P)$ so that in neighborhoods of $(0,0)$ and $\Phi(0,0)$ we have*

$$(P,Q) = \Phi(p,q) \quad \Longleftrightarrow \quad p = \frac{\partial W}{\partial q}, \quad Q = \frac{\partial W}{\partial P}. \tag{8.1}$$

Moreover, we have $\det \frac{\partial^2 W}{\partial P \partial q} \neq 0$.

(b) *Conversely, if $W(q,P)$ is smooth and* $\det \frac{\partial^2 W}{\partial P \partial q} \neq 0$*, then* (8.1) *defines a canonical transformation between neighborhoods of $(0,0)$ and $\Phi(0,0)$.*

Proof. (a) We claim that there exists a function $V(p,q)$ so that

$$\nabla V = \begin{pmatrix} \frac{\partial V}{\partial p_i} \\ \frac{\partial V}{\partial q_i} \end{pmatrix} = \begin{pmatrix} \sum_j Q_j \frac{\partial P_j}{\partial p_i} \\ \sum_j Q_j \frac{\partial P_j}{\partial q_i} \end{pmatrix} + \begin{pmatrix} \sum_j p_j \frac{\partial q_j}{\partial p_i} \\ \sum_j p_j \frac{\partial q_j}{\partial q_i} \end{pmatrix} = \begin{pmatrix} \sum_j Q_j \frac{\partial P_j}{\partial p_i} \\ \sum_j Q_j \frac{\partial P_j}{\partial q_i} \end{pmatrix} + \begin{pmatrix} 0 \\ p_i \end{pmatrix}. \tag{8.2}$$

For (8.2) to hold, we simply check the equality of mixed partials. We will verify this for one example:

$$\frac{\partial^2 V}{\partial q_k \partial q_i} = \frac{\partial}{\partial q_k}\left[\sum_{j=1}^n Q_j \frac{\partial P_j}{\partial q_i} + p_i\right] = \sum_{j=1}^n \left(\frac{\partial Q_j}{\partial q_k}\frac{\partial P_j}{\partial q_i} + Q_j \frac{\partial^2 P_j}{\partial q_k \partial q_i}\right),$$
$$\frac{\partial^2 V}{\partial q_i \partial q_i k} = \frac{\partial}{\partial q_i}\left[\sum_{j=1}^n Q_j \frac{\partial P_j}{\partial q_k} + p_k\right] = \sum_{j=1}^n \left(\frac{\partial Q_j}{\partial q_i}\frac{\partial P_j}{\partial q_k} + Q_j \frac{\partial^2 P_j}{\partial q_i \partial q_k}\right).$$

Note that the second terms on the RHS agree. As Φ is canonical, then by Proposition 7.20 we know that

$$\Phi' = \begin{pmatrix} \frac{\partial P}{\partial p} & \frac{\partial P}{\partial q} \\ \frac{\partial Q}{\partial p} & \frac{\partial Q}{\partial q} \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

is a symplectic matrix, and so the blocks satisfy (cf. (7.20))

$$A^T C = C^T A, \quad B^T D = D^T B, \quad A^T D - C^T B = I.$$

This first relation implies

$$\sum_{j=1}^n \frac{\partial Q_j}{\partial q_k}\frac{\partial P_j}{\partial q_i} = A^T C = C^T A = \sum_{j=1}^n \frac{\partial Q_j}{\partial q_i}\frac{\partial P_j}{\partial q_k},$$

which demonstrates the equality of mixed partials for $\frac{\partial^2 V}{\partial q_k \partial q_i}$ and $\frac{\partial^2 V}{\partial q_i \partial q_k}$. (The second relation $B^T D = D^T B$ is needed for $\frac{\partial^2 V}{\partial p_i \partial p_k}$ and the third relation $A^T D - C^T B = I$ for $\frac{\partial^2 V}{\partial p_i \partial q_k}$.) In fact, this demonstrates that (8.2) is locally solvable by some V if and only if Φ is canonical.

Next, as $\det \frac{\partial P}{\partial p} \neq 0$, the implicit function guarantees that $(p, q) \mapsto (P, q)$ is a local diffeomorphism. Therefore we may define

$$W(q, P) = V(q, p(q, P)).$$

It remains to check that the relations (8.1) hold so that W is the generating function for Φ. To emphasize that we are working with the coordinates (P, q), we may write this as

$$p = \left(\frac{\partial W}{\partial q}\right)_P, \qquad Q = \left(\frac{\partial W}{\partial P}\right)_q.$$

Think of (8.2) as an equality of directional derivatives. (Indeed, in differential geometry notation we would write (8.2) as $Q\,\mathrm{d}P + p\,\mathrm{d}q = \mathrm{d}V$.) We plug in the direction $(\frac{\partial}{\partial q_k})_P$ into (8.2) to obtain

$$\left(\frac{\partial W}{\partial q_k}\right)_P = \frac{\partial V}{\partial q_k} = 0 + p_k.$$

Likewise, $(\frac{\partial}{\partial P_k})_q$ yields

$$\left(\frac{\partial W}{\partial P_k}\right)_q = \frac{\partial V}{\partial P_k} = Q_k + 0.$$

(b) Given $W(q, P)$ smooth such that $\det \frac{\partial^2 W}{\partial P \partial q} \neq 0$, the implicit function theorem guarantees that $(P, q) \mapsto (p, q)$ for $p = \frac{\partial W}{\partial q}$ is a local diffeomorphism. In particular, $Q = \frac{\partial W}{\partial P}$ can be written as a smooth function of p, q.

To verify that $(p, q) \mapsto (P, Q)$ is canonical, it suffices to check that (8.2) holds for W. This is a straightforward computation using the values of the partial derivatives guaranteed by the implicit function theorem. □

8.2. Local structure of Hamiltonian flows

We would like to understand the structure of a Hamiltonian flow in a neighborhood of a point up to changes in coordinates. Given an arbitrary Poisson structure $J(x)$ and a point x_0, we may choose canonical coordinates on a neighborhood of x_0 by the Darboux theorem (Theorem 7.18). If there are Casimirs, we can restrict our attention to one of their level sets so that the flow takes the form

$$\dot{x} = J\nabla H, \qquad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \tag{8.3}$$

First, consider the case where $\nabla H(x_0) \neq 0$. From the general theory of ODEs (cf. Proposition A.18) this implies that there is a choice of coordinates so that the flow is uniform, but we can say something more specific about our Hamiltonian ODE. In our proof of Theorem 7.18, we can make any choice for

the first coordinate p_1, like $p_1 = H$. Therefore, we can construct local canonical coordinates $(H, p_2, \dots, p_n, q_1, \dots, q_n)$, and our flow is then

$$\dot{q}_1 = p_1, \quad \dot{p}_1 = 0, \quad \dot{q}_i = \dot{p}_i = 0 \quad \text{for } i = 2, \dots, n.$$

Next, consider the case of a fixed point $\nabla H(x_0) = 0$. After translating, we may assume that $x_0 = 0$. The standard procedure in the theory of ODEs (cf. section A.6) is to linearize:

$$\dot{y} = \big[JH''(0)\big]y. \tag{8.4}$$

This is a Hamiltonian flow for the quadratic Taylor approximation of our Hamiltonian:

$$H(0) + \tfrac{1}{2}x \cdot H''(0)x. \tag{8.5}$$

We will study quadratic Hamiltonians in finer detail in section 8.3.

For general ODEs, the Hartman–Grobman theorem (Theorem A.21) tells us that if the matrix for the linearized flow (8.4) has no purely imaginary eigenvalues, then the actual flow (8.3) is qualitatively determined by the spectrum of the matrix for the linearized flow. For Hamiltonian flows, the matrix in (8.4) must be of the form $JH''(0)$ for $H''(0)$ real and symmetric, and so we have some conditions on the spectrum:

Proposition 8.2. *The linearized equation* (8.4) *has the following properties.*

(a) A complex number $\lambda \in \mathbb{C}$ is a eigenvalue for $JH''(0)$ if and only if $\overline{\lambda}$ is, and $\lambda, \overline{\lambda}$ have equal algebraic and geometric multiplicities.

(b) A complex number $\lambda \in \mathbb{C}$ is a eigenvalue for $JH''(0)$ if and only if $-\lambda$ is, and $\lambda, -\lambda$ have equal algebraic and geometric multiplicities.

(c) The linear flow map $e^{tJH''(0)}$ is a symplectic matrix for every $t \in \mathbb{R}$.

Note that property (b) tells us that the trace of $JH''(0)$ is zero, and so the linear flow map $e^{tJH''(0)}$ preserves volume in phase space. This must be the case by Liouville's theorem (Proposition 7.23), since the linear flow is Hamiltonian for the Hamiltonian (8.5).

Proof. (a) This is because the matrix $JH''(0)$ is real.

(b) Let $\sigma(JH''(0))$ denote the spectrum of $JH''(0)$. As $H''(0)$ is symmetric, we have

$$\begin{aligned}\sigma\big(JH''(0)\big) &= \sigma\big([JH''(0)]^T\big) = \sigma\big(-H''(0)J\big) \\ &= \sigma\big(J[-H''(0)J]J^{-1}\big) = \sigma\big(-JH''(0)\big).\end{aligned}$$

(c) This is because the linear flow is Hamiltonian for the Hamiltonian (8.5). Indeed, the flow map for a Hamiltonian flow is a canonical transformation by Proposition 7.24, and for the canonical Poisson bracket this simply means that the derivative of $e^{tJH''(0)}$ is a symplectic matrix by Proposition 7.20. □

While property (c) tells us that $e^{tJH''(0)}$ is always a symplectic matrix, not every symplectic matrix admits the representation $e^{tJH''(0)}$ for a symmetric matrix $H''(0)$. For example, the matrix

$$\begin{pmatrix} -4 & 0 \\ 0 & -\frac{1}{4} \end{pmatrix} \tag{8.6}$$

is symplectic, and it cannot be written as $e^{tJH''(0)}$ since then it would admit a real square root $e^{tJH''(0)/2}$; this root would then have eigenvalues $\pm 2i$ and $\pm\frac{1}{2}i$, which is too many. (Note that this example is not near the identity, while $e^{tJH''(0)}$ tends towards the identity as $t \to 0$.) On the other hand, it can be shown that the polar decomposition matrices of a symplectic matrix are symplectic, and so it follows that every symplectic matrix is the product of two matrices of the form $e^{tJH''(0)}$.

8.3. Normal forms for quadratic Hamiltonians

In this section, we seek a global understanding of the flow for quadratic Hamiltonians. As in the beginning of section 8.2, it suffices to consider the canonical Poisson bracket. At the end of the section we will turn to a discussion of the general case, but first we will study the important case of the Hamiltonian

$$H = \tfrac{1}{2} \sum_{i,j=1}^{n} M_{ij}^{-1} p_i p_j + \tfrac{1}{2} \sum_{i,j=1}^{n} V_{ij} q_i q_j \tag{8.7}$$

for M a positive definite matrix and V a symmetric matrix. We call M the mass matrix so that the first term on the RHS is the kinetic energy, and the second term is the potential energy landscape.

Such a system arises naturally in practice. Consider a system of particles with Hamiltonian

$$H = \sum_{i=1}^{n} \tfrac{1}{2m_i} p_i^2 + \tfrac{1}{2} \sum_{i<j} U(q_i - q_j).$$

For such a system, the total momentum $P = \sum p_i$ is conserved because H is invariant under a collective translation; this follows from Proposition 1.13 or a simple computation. Consequently, it suffices to study the motion from the center of mass frame, where $P = 0$ and the center of mass $Q = (\sum m_i q_i)/(\sum m_i)$ is conserved. As we now have $P = 0$, we might eliminate one p_i, say, $p_n = -p_1 - \cdots - p_{n-1}$. In this way, mass matrices arise naturally. Quadratic potential energies frequently arise as Taylor approximations for more general systems, and the behaviors that arise from this special case is fundamental to understanding the general case.

We would like to boil down the Hamiltonian (8.7) to its essential parts in order to obtain a simple description of its flow. A first step is to make the mass matrix go away, via the canonical change of variables

$$p_{\text{new}} = M^{-\frac{1}{2}} p_{\text{old}}, \qquad q_{\text{new}} = M^{\frac{1}{2}} q_{\text{old}}.$$

Here, we take the self-adjoint square root $M^{\frac{1}{2}}$. This is a canonical transformation because the matrix

$$\begin{pmatrix} A & 0 \\ 0 & A^{-T} \end{pmatrix}$$

is symplectic whenever A is invertible (which is easily verified using (7.20)). In the new variables, the Hamiltonian (8.7) becomes

$$H = \tfrac{1}{2}|p|^2 + \tfrac{1}{2} q \cdot \widetilde{V} q \tag{8.8}$$

for the new symmetric matrix $\widetilde{V} = M^{-\frac{1}{2}} V M^{-\frac{1}{2}}$.

Next, we diagonalize $\widetilde{V}$:

$$\widetilde{V} = O \begin{pmatrix} \kappa_1 & & \\ & \ddots & \\ & & \kappa_d \end{pmatrix} O^T,$$

where O is an orthogonal matrix. Consider the canonical change of variables

$$p_{\text{new}} = O^T p_{\text{old}}, \qquad q_{\text{new}} = O^T q_{\text{old}}.$$

This turns the Hamiltonian (8.8) into

$$H = \tfrac{1}{2} \sum_{i=1}^{n} (p_i^2 + \kappa_i q_i^2). \tag{8.9}$$

Altogether, we have reduced the general quadratic system (8.7) to a system of decoupled one-dimensional particles.

If $\kappa_i > 0$, then we set $\omega^2 = \kappa_i$. The Hamiltonian for the ith particle is then

$$H_i = \tfrac{1}{2} p^2 + \tfrac{1}{2} \omega^2 q^2,$$

which is the harmonic oscillator of Example 2.2. Indeed, the equations of motion take the form

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = J H''(0) \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\omega^2 & 0 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}.$$

From its trace and determinant, we see that the that the matrix on the RHS has eigenvalues $\pm i\omega$. The trajectories in phase space are ellipses due to the conservation of H. In fact, we can perform one further canonical change of variables

$$p_{\text{new}} = \omega^{-\frac{1}{2}} p_{\text{old}}, \qquad q_{\text{new}} = \omega^{\frac{1}{2}} q_{\text{old}}$$

to symmetrize the Hamiltonian

$$H_i = \tfrac{\omega}{2} (p_i^2 + q_i^2) \tag{8.10}$$

so that the trajectories are circular.

If $\kappa_i < 0$, then we set $\gamma^2 = -\kappa_i$. Then the ith Hamiltonian is

$$H_i = \tfrac{1}{2}p^2 - \tfrac{1}{2}\gamma^2 q^2,$$

which is the saddle node of Example 2.1. The equations of motion are

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ \gamma^2 & 0 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix},$$

and the matrix on the RHS has eigenvalues $\pm\gamma$. The trajectories in phase space trace out the hyperbolic level sets of H_i. To symmetrize the Hamiltonian, we can take the canonical change of variables

$$p_{\text{new}} = \gamma^{-\frac{1}{2}} p_{\text{old}}, \qquad q_{\text{new}} = \gamma^{\frac{1}{2}} q_{\text{old}}$$

to make

$$H_i = \tfrac{\gamma}{2}(p_i^2 - q_i^2).$$

Alternatively, the canonical change variables

$$\begin{pmatrix} p_{\text{new}} \\ q_{\text{new}} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -\gamma \\ \gamma^{-1} & 1 \end{pmatrix} \begin{pmatrix} p_{\text{old}} \\ q_{\text{old}} \end{pmatrix}$$

makes

$$H_i = \gamma p_i q_i. \tag{8.11}$$

Lastly, in the case $\kappa_i = 0$ we have

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix},$$

a 2×2 Jordan block with eigenvalue zero. The Hamiltonian

$$H_i = \tfrac{1}{2}p_i^2 \tag{8.12}$$

is shaped like a trough. Consequently, the origin is a non-isolated fixed point that is not Lyapunov stable; trajectories are straight linear of constant p (and $q(t) = q_0 + tp_0$). This is called rectilinear motion (or sometimes secular drift).

Altogether, we notice that notice that if the potential energy is bowl-shaped in the sense that all κ_i are positive, then the fixed point at the origin is Lyapunov stable. If one κ_i is nonpositive, then the fixed point at the origin is not Lyapunov stable. Moreover, eigenvalues $\gamma \pm i\omega$ with both $\gamma, \omega \neq 0$ do not occur for such Hamiltonians.

More generally, H bowl-shaped implies that the fixed point at the bottom is Lyapunov stable:

Theorem 8.3 (Dirichlet–Lagrange)**.** *If the Hamiltonian H has a critical point at x_0 and the Hessian matrix $H''(x_0)$ is positive definite, then x_0 is a Lyapunov stable fixed point for Hamilton's equations* (7.15)*.*

Proof. This follows immediately from the fact that H is a (weak) Lyapunov function (cf. Lemma 2.8) and Theorem 2.10. □

As a warning, it is false that a not bowl-shaped Hamiltonian implies that the the fixed point is unstable. Indeed, saddle-shaped Hamiltonians can have stable fixed points. For example, the Hamiltonian

$$H = \tfrac{1}{2}(p_1^2 + q_1^2) - \tfrac{1}{2}(p_2^2 + q_2^2)$$

consists of a harmonic oscillator in the first variables, and a time-reversed harmonic oscillator in the second variables. In order to determine stability, the key is how the saddle directions interact with the symplectic structure.

Altogether, we have seen 3 normal forms: (8.10), (8.11), and (8.12). These are normal forms in the sense that given a Hamiltonian of the form (8.7), there is a linear canonical transformation decomposing into a direct sum (cf. (8.9)) of these 3 forms. For general quadratic Hamiltonians, we have the following result based on the work of Williamson [Wil36]:

Theorem 8.4 (Williamson's theorem)**.** *Given a nondegenerate Poisson bracket, there are 9 normal forms so that for any quadratic Hamiltonian there exists a canonical transformation which decomposes it into a direct sum of these forms.*

For a complete list of these canonical forms, see [Arn89, App. 6].

It is indeed possible to have complex eigenvalues $\gamma + i\omega$ with both $\gamma, \omega \neq 0$. For example, consider the Hamiltonian

$$H = \gamma(p_1 q_1 + p_2 q_2) + \omega(p_1 q_2 - p_2 q_1)$$

which consists of a saddle in the first and second variables plus an interaction term. This leads to the linear ODE with matrix

$$JH'' = \begin{pmatrix} \gamma & \omega & 0 & 0 \\ -\omega & \gamma & 0 & 0 \\ 0 & 0 & -\gamma & \omega \\ 0 & 0 & -\omega & -\gamma \end{pmatrix}$$

(in terms of the ordered basis (q_1, q_2, p_1, p_2)), which has eigenvalues $\pm\gamma \pm i\omega$. As a side note, if we take $\gamma = \log 4$ and $\omega = \pi$ then we obtain

$$e^{JH''} = \begin{pmatrix} -4 & & & \\ & -4 & & \\ & & -\frac{1}{4} & \\ & & & -\frac{1}{4} \end{pmatrix}.$$

Recall that the 2-dimensional version (8.6) of this matrix could not be expressed in such an exponential form.

8.4. Birkhoff normal form

Let H be a Hamiltonian that is real analytic with a fixed point at the origin. We seek to simplify the structure of H near the origin via a smooth and canonical change of variables. As in the beginning of section 8.2, it suffices to consider the canonical Poisson bracket.

In section 8.3, we saw how to reduce the quadratic part of the Hamiltonian to a normal form. Consequently, we now seek a nonlinear change of variables (near the identity) to reduce the complexity of the nonlinear terms. The method we will present is iterative, in the sense that we tidy up the terms in the Taylor expansion one order at a time.

Inductively assume that we have treated the Taylor expansion up to order $k-1$ for some $k \geq 3$. We will prescribe a canonical transformation via a generating function $W(P,q)$ of the form discussed in section 8.1. Our generating function will be of the form

$$W(P,q) = Pq + F(P,q), \tag{8.13}$$

where the first term Pq which generates the identity, and the error F is a polynomial that is homogeneous of degree k. The transformation generated by (8.13) is

$$p = P + \frac{\partial F}{\partial q}(P,q), \qquad Q = q + \frac{\partial F}{\partial P}(P,q). \tag{8.14}$$

These coordinates are guaranteed to be a local diffeomorphism near the origin because the leading term is the identity and the remainders above are degree 2 or higher. Rearranging (8.14), we have

$$\begin{aligned} P &= p - \frac{\partial F}{\partial q}(p,q) + \left[\frac{\partial F}{\partial q}(p,q) - \frac{\partial F}{\partial q}(P,q)\right] \\ &= p - \frac{\partial F}{\partial q}(p,q) + \left[\frac{\partial F}{\partial q}(p,q) - \frac{\partial F}{\partial q}\left(p - \frac{\partial F}{\partial q}, q\right)\right]. \end{aligned}$$

Note that the input for the first $\frac{\partial F}{\partial q}$ on the RHS is p and not P; we are treating F here as a mathematical function here (rather than an observable) and inserting p in place of P without changing the formula for F. As F is a homogeneous polynomial of degree $k \geq 3$, then the square-bracketed term on the RHS is of degree at least $2k-3 \geq k$ in p, q, and thus is higher order than the first terms:

$$P = p - \frac{\partial F}{\partial q}(p,q) + \mathcal{O}\big(|p|^k + |q|^k\big). \tag{8.15}$$

Similarly, we have

$$Q = q + \frac{\partial F}{\partial p}(p,q) + \mathcal{O}\big(|p|^k + |q|^k\big). \tag{8.16}$$

We are now prepared to perform our change of variables. Taylor expand

$$H = H_2 + H_3 + \cdots + H_k + \ldots,$$

where H_n is a homogeneous polynomial of degree n. We may assume that $H_0 = 0$ after adding a constant to our Hamiltonian, and $H_1 = 0$ since the origin is a fixed point. Let $\Phi(p,q) = (P,Q)$ be the canonical transformation associated to the generating function W. By (8.15) and (8.16), the leading order of this transformation yields

$$H \circ \Phi(p,q) = H_2(p,q) + \cdots + H_{k-1}(p,q) + \left[H_k + \frac{\partial H_2}{\partial q} \cdot \frac{\partial F}{\partial p} - \frac{\partial H_2}{\partial p} \cdot \frac{\partial F}{\partial q}\right](p,q) + \mathcal{O}\big(|p|^{k+1} + |q|^{k+1}\big).$$

We conclude that the transformation Φ leaves the terms $H_2, \ldots, H_{k-1}$ that have already been accounted for untouched, and replaces H_k by $H_k + \{H_2, F\}$. It also changes all of the higher order terms, but these are computable to any finite degree.

It remains to show that we can pick F so that $\{H_2, F\}$ cancels H_k. We will examine how to do this for the examples of normal forms that we saw in section 8.3.

8.4.1. Hyperbolic case. Suppose that H_2 can be fully decomposed into the direct sum of the normal form (8.11):

$$H_2 = \sum_{j=1}^{n} \gamma_j p_j q_j. \tag{8.17}$$

We write

$$F = \sum_{|\alpha+\beta|=k} f_{\alpha\beta} p^\alpha q^\beta,$$

where the sum ranges over multiindices $\alpha, \beta \in \mathbb{N}^n$, we use the notations $p^\alpha = p^{\alpha_1} \cdots p_n^{\alpha_n}$ and $|\alpha| = \sum |\alpha_j|$, and we take coefficients $f_{\alpha\beta} \in \mathbb{R}$. We compute

$$\begin{aligned}
\{H_2, F\} &= \sum_{\alpha,\beta} f_{\alpha\beta} \sum_{j=1}^{n} \left[\frac{\partial H_2}{\partial q_j}\frac{\partial}{\partial p_j}(p^\alpha q^\beta) - \frac{\partial H_2}{\partial p_j}\frac{\partial}{\partial q_j}(p^\alpha q^\beta)\right] \\
&= \sum_{\alpha,\beta} f_{\alpha\beta} \sum_{j=1}^{n} \big[\gamma_j \alpha_j - \gamma_j \beta_j\big] p^\alpha q^\beta \\
&= \sum_{\alpha,\beta} \gamma \cdot (\alpha - \beta) f_{\alpha\beta} p^\alpha q^\beta,
\end{aligned}$$

where $\gamma = (\gamma_1, \ldots, \gamma_n)$. Consequently, we may cancel any term $h_{\alpha\beta} p^\alpha q^\beta$ in H_k by setting

$$f_{\alpha\beta} = -\frac{h_{\alpha\beta}}{\gamma \cdot (\alpha - \beta)}, \tag{8.18}$$

provided that $\gamma \cdot (\alpha - \beta) \neq 0$. In particular, we cannot eliminate terms with $\alpha = \beta$. The best case scenario is when γ is **nonresonant of degree** k:

$$\sum_{i=1}^{n} k_i \gamma_i \neq 0 \quad \text{for all } k_1, \ldots, k_n \in \mathbb{Z} \text{ such that } 0 < \sum |k_i| \leq k,$$

then all terms with $\alpha \neq \beta$ can be canceled. If γ is resonant, then we can still apply this method to remove all nonresonant terms; note that we did not assume that $H_3, \ldots, H_{k-1}$ were in normal form, and so the presence of surviving resonant terms is okay. This leaves us with a *resonant normal form*, which is still simpler than the original Hamiltonian. As $\gamma \cdot (\alpha - \beta)$ appears in the denominator of (8.18), we see that when $\gamma \cdot (\alpha - \beta)$ is small then we must choose $f_{\alpha\beta}$ large—this resonance phenomenon is called *small denominators*.

Suppose that γ is nonresonant of degree k. Then for all $\alpha \neq \beta$ we may prescribe the coefficients of F according to (8.18). This yields a canonical change of variables in a neighborhood of the origin which turns H into

$$H = H_2(p,q) + \sum_{j=3}^{k} \sum_{|\alpha|=j} c_\alpha p^\alpha q^\alpha + \mathcal{O}\big(|p|^{k+1} + |q|^{k+1}\big).$$

Setting

$$I_j = p_j q_j,$$

we see that all of the terms above are functions only of the I_j:

$$H = h(I_1, \ldots, I_n) + \mathcal{O}\big(|p|^{k+1} + |q|^{k+1}\big). \tag{8.19}$$

As I_j depends only on the jth variables, then we have

$$\{I_j, I_k\} = 0 \quad \text{for all } j, k. \tag{8.20}$$

Thus

$$\begin{aligned} \dot{I}_j = \{I_j, H\} &= \{I_j, h(I_1, \ldots, I_n)\} + \big\{I_j, \mathcal{O}\big(|p|^{k+1} + |q|^{k+1}\big)\big\} \\ &= \mathcal{O}\big(|p|^{k+1} + |q|^{k+1}\big) = \mathcal{O}\big(|I_1|^{\frac{k+1}{2}} + \cdots + |I_n|^{\frac{k+1}{2}}\big), \end{aligned} \tag{8.21}$$

and so the I_j are almost conserved by the flow for k large.

8.4.2. Elliptic case. Suppose that H_2 can be fully decomposed as the direct sum of the normal form (8.10):

$$H_2 = \sum_{j=1}^{n} \tfrac{1}{2}\omega_j (p_j^2 + q_j^2). \tag{8.22}$$

It turns out that the computation is more elegant in terms of the complex variables

$$z_j = p_j + iq_j, \qquad \overline{z}_j = p_j - iq_j$$

so that

$$H_2 = \sum_{j=1}^{n} \tfrac{1}{2}\omega_j z_j \overline{z}_j,$$

even though our final choice of canonical transformation will be real. Note that complex polynomials in p_j, q_j correspond to complex polynomials in $z_j, \overline{z}_j$. We also extend the bracket $\{\cdot,\cdot\}$ to be bilinear (as opposed to Hermitian), so that

$$\{z_j, z_k\} = 0, \qquad \{\overline{z}_j, \overline{z}_k\} = 0, \qquad \{z_j, \overline{z}_k\} = 2i\delta_{jk}.$$

We write

$$F = \sum_{|\alpha+\beta|=k} f_{\alpha\beta} z^\alpha \overline{z}^\beta,$$

with the requirement that $f_{\beta\alpha} = \overline{f_{\alpha\beta}}$ so that F is real-valued. Using the product rule (cf. Definition 7.7), we compute

$$\begin{aligned}
\{H_2, F\} &= \sum_{\alpha,\beta} f_{\alpha\beta} \sum_{j=1}^n \tfrac{1}{2}\omega_j \{z_j\overline{z}_j, z^\alpha \overline{z}^\beta\} \\
&= \sum_{\alpha,\beta} f_{\alpha\beta} \sum_{j=1}^n \tfrac{1}{2}\omega_j \big[z_j\{\overline{z}_j, z^\alpha\overline{z}^\beta\} + \overline{z}_j\{z_j, z^\alpha\overline{z}^\beta\}\big] \\
&= \sum_{\alpha,\beta} f_{\alpha\beta} \sum_{j=1}^n \tfrac{1}{2}\omega_j \big[-2i\alpha_j + 2i\beta_j\big] z^\alpha\overline{z}^\beta \\
&= -i\sum_{\alpha,\beta} \omega\cdot(\alpha-\beta) f_{\alpha\beta} z^\alpha\overline{z}^\beta,
\end{aligned}$$

where $\omega = (\omega_1, \ldots, \omega_n)$. Consequently, we may cancel any term $h_{\alpha\beta} z^\alpha \overline{z}^\beta$ in H_k by setting

$$f_{\alpha\beta} = \frac{i h_{\alpha\beta}}{\omega\cdot(\alpha-\beta)}, \tag{8.23}$$

whenever $\omega\cdot(\alpha-\beta) \neq 0$. Note that as H_k is real-valued, then these coefficients automatically satisfy the reality condition $f_{\beta\alpha} = \overline{f_{\alpha\beta}}$.

We conclude that if ω is nonresonant of degree k then we may eliminate (using a *real-valued* change of variables) all terms of H_k with $\alpha \neq \beta$, leaving

$$H = H_2(p,q) + \sum_{j=3}^k \sum_{|\alpha|=j} c_\alpha z^\alpha \overline{z}^\alpha + \mathcal{O}\big(|p|^{k+1} + |q|^{k+1}\big).$$

Setting

$$I_j = \tfrac{1}{2} z_j \overline{z}_j = \tfrac{1}{2}(p_j^2 + q_j^2),$$

we obtain

$$H = h(I_1, \ldots, I_n) + \mathcal{O}\big(|p|^{k+1} + |q|^{k+1}\big). \tag{8.24}$$

Moreover, the variables I_j still satisfy the bracket relations (8.20) and are almost conserved by the flow in the sense of (8.21).

8.5. Completely integrable systems

Suppose that we have a Hamiltonian whose quadratic part is of the elliptic type (8.22), and assume that the Birkhoff normal form produces a convergent change of variables as $k \to \infty$. This is a strong assumption, as it requires that the coefficients $f_{\alpha\beta}$ of the kth generating function F_k decay sufficiently rapidly as $k \to \infty$. In the formulas (8.18) and (8.23) we saw that the frequencies ω of the quadratic normal form appear in the denominator as the term $\omega \cdot (\alpha - \beta)$. These denominators will not vanish provided that ω is nonresonant of all degrees, but they still may be very small rather often. (This is closely related to the concepts of Diophantine and Liouville numbers in number theory.)

Under this assumption, by taking $k \to \infty$ in (8.24) our new Hamiltonian is of the form

$$H = h(I_1, \dots, I_n) \tag{8.25}$$

with $h(0) = 0$ and $\nabla h(0) = \omega$. Moreover, the new variables $I_j = \frac{1}{2}(p_j^2 + q_j^2)$ are in **involution** (or **Poisson commute**) with each other:

$$\{I_j, I_k\} = 0 \quad \text{for all } j, k. \tag{8.26}$$

Together with (8.25), this implies that the quantities I_j are conserved:

$$\dot{I}_j = \{I_j, H\} = 0 \quad \text{for all } j. \tag{8.27}$$

When we have a set of n functionally independent quantities satisfying (8.26) and (8.27), we say that the Hamiltonian flow of H is **completely integrable**. (The condition that the I_j are functionally independent is intentionally a little vague, but it is essential and will be made concrete in each rigorous statement that we make.) Note that canonical transformations preserve complete integrability, and so the Hamiltonian flow of H remains completely integrable even after we undo the Birkhoff normal form transformation.

To fill out these quantities into a complete set of coordinates, we define

$$\phi_j = \arg(p_j + iq_j) \in \mathbb{R} \quad \text{for } p_j + iq_j \in \mathbb{C} \setminus \{0\}.$$

A direct computation shows that these variables satisfy the relations

$$\{\phi_j, \phi_k\} = 0, \quad \{\phi_j, I_k\} = \delta_{jk} \quad \text{for all } j, k. \tag{8.28}$$

Together, we obtain a complete set of coordinates satisfying the following properties.

Definition 8.5. Coordinates (ϕ, I) on $\mathbb{R}^{2n}$ are **action-angle coordinates** for the Hamiltonian H if:

(a) They satisfy the canonical relations (8.26) and (8.28),

(b) The Hamiltonian $H = h(I_1, \dots, I_n)$ is a function of only $I_1, \dots, I_n$,

(c) The **action coordinates** I_j are conserved and the **angle coordinates** ϕ_j evolve linearly in time:

$$\dot{I}_j = 0, \qquad \dot{\phi}_j = \frac{\partial h}{\partial I_J}(I_1, \ldots, I_n) = \text{constant}$$

for all j.

So far, we have seen that in the elliptic case, if the Birkhoff normal form converges as $k \to \infty$ then the system is completely integrable and we can find a set of action-angle coordinates. This can also be done in the hyperbolic case (8.17) and other cases as well, although the angle coordinate is no longer corresponds to an actual angle. (For example, for the free Hamiltonian (8.12) with rectilinear motion the angle coordinate $q(t) = q_0 + tp_0$ traces out a straight line.) As it turns out, the converse is also true: if a system is completely integrable, then the Birkhoff normal forms converge.

For the remainder of this section, we will abandon the ellipticity and normal form assumptions and consider a general completely integrable Hamiltonian H. By definition, the existence of action-angle coordinates immediately implies that the system is completely integrable. The converse is also true: if a system is completely integrable then *formally* we may find action-angle coordinates. This process is called **Liouville integration**, as the action-angle coordinates provide parametric solutions to the equations of motion.

It should be noted that completely integrable systems are quite exceptional within the class of Hamiltonian systems. Specifically, Siegel [Sie54] showed that generic (in the sense of the Baire category theorem) analytic Hamiltonians in a neighborhood of a fixed point are not integrable.

Nevertheless, complete integrability is general enough to include a rich family of examples. In addition to the Birkhoff normal form example at the beginning of this section (and the Toda lattice system that we will study in section 8.6), we have the following two examples.

Example 8.6 (One-dimensional systems)**.** Every conservative system with one degree of freedom:

$$E = \tfrac{1}{2}m\dot{x}^2 + V(x), \quad x \in \mathbb{R}$$

is completely integrable. Indeed, phase space is two-dimensional and so this total energy provides the one conserved quantity that we require. Rearranging this conservation law, we are able to replace the second-order equation of motion with the first-order equation

$$\dot{x} = \pm\sqrt{\tfrac{2}{m}[E - V(x)]},$$

which is separable and thus provides a formal solution for the motion. Even without explicitly evaluating this integral, we were able to use this formula in section 2.5 to draw many conclusions (Propositions 2.16, 2.18 and 2.19).

Example 8.7 (Central fields)**.** A particle in $\mathbb{R}^3$ moving under the influence of a radial potential:

$$H = \tfrac{1}{2m}|\mathbf{p}|^2 + V(|\mathbf{x}|), \qquad \mathbf{x} \in \mathbb{R}^3$$

is completely integrable. As phase space is six-dimensional, this requires three conserved quantities. Spherical symmetry tells us that the 3 components of the angular momentum $\mathbf{L} = \mathbf{x} \times \mathbf{p}$ are conserved (cf. Proposition 1.16). However, these quantities are not in involution! Indeed, we have

$$\{L_1, L_2\} = L_3, \qquad \{L_2, L_3\} = L_1, \qquad \{L_3, L_1\} = L_2,$$

which expresses the fact that the components of the angular momentum provide a representation of the Lie algebra of the rotation group $SO(3)$.

Nevertheless, this system is completely integrable. It is straightforward to check that the three functionally independent quantities

$$H, \quad |\mathbf{L}|^2, \quad L_3$$

are in involution. In section 3.1, we used this to replace the second-order equations of motion with first-order equations, which we could integrate to obtain a formal solution (cf. (3.5) and (3.6)).

For the Kepler potential

$$V(r) = -k|\mathbf{x}|^{-1}, \quad k \neq 0$$

we know that all bounded orbits are closed. However, the 4 conserved quantities $H, \mathbf{L}$ only tell us that orbits are constrained to a two-dimensional surface and hence may not be—and in general are not—closed (cf. Theorem 3.3). For the Kepler potential, Laplace discovered that

$$\mathbf{A} = \mathbf{L} \times \mathbf{p} + k\frac{\mathbf{x}}{|\mathbf{x}|}$$

is also conserved. Now we have 7 conserved quantities, which is too many! It turns out that there are exactly 2 redundancies:

$$\mathbf{L} \cdot \mathbf{A} = 0, \qquad |\mathbf{A}|^2 = 2H|\mathbf{L}|^2 + k^2.$$

This leaves us with 5 functionally independent conserved quantities, which implies that trajectories are restricted to a one-dimensional manifold as desired.

The Poisson brackets of these 5 quantities can also be computed, and it turns out that they provide a representation of the *four*-dimensional rotation group $SO(4)$. Moser (cf. [MZ05, §1.6]) explained this symmetry by showing that for negative energy, the Kepler problem is diffeomorphic to geodesic motion on the sphere $S^3 \subset \mathbb{R}^4$.

These examples illustrate the procedure of Liouville integration: when a system is completely integrable, there are enough conserved quantities so that we may integrate the equations of motion and find a formal expression for the solution. In practice, the exact procedure varies from system to system. Nevertheless, we have the following general fact:

Theorem 8.8 (Liouville–Arnold–Jost)**.** *Suppose that $F_1, \dots, F_n : \mathbb{R}^{2n} \to \mathbb{R}$ are smooth and $\{x \in \mathbb{R}^{2n} : \mathbf{F}(x) = \boldsymbol{c}_0\}$ is a smooth compact connected n-dimensional manifold on which $\nabla F_1, \dots, \nabla F_n$ are linearly independent. If the F_i are also in involution with each other, then there exist action-angle coordinates $\boldsymbol{\phi} \in \mathbb{R}^n/2\pi\mathbb{Z}^n$, $\boldsymbol{I} \in \mathbb{R}^n$ so that the canonical relations* (8.26) *and* (8.28) *hold, $\boldsymbol{I} \equiv \boldsymbol{I}(F_1, \dots, F_n)$ is a function only of $\mathbf{F}$, and $\boldsymbol{I}$ is a smooth local diffeomorphism near $\boldsymbol{c}_0$.*

We partially attribute this result to Liouville, as he founded the idea of Liouville integration. Arnold was the first to make this rigorous statement on $\mathbb{R}^{2n}$, and Jost extended the result to general manifolds.

Topologically, we interpret Theorem 8.8 as saying that we have a foliation of $\mathbb{R}^{2n}$ by tori in a way that respects the Poisson structure. Indeed, $(\boldsymbol{\phi}, \mathbf{I})$ provides a map from a neighborhood of $\{\mathbf{F} = \mathbf{c}_0\}$ in $\mathbb{R}^{2n}$ into $\mathbb{R}^n/2\pi\mathbb{Z}^n \times \{\mathbf{c} \in \mathbb{R}^n : |\mathbf{c} - \mathbf{c}_0| < \epsilon\}$. For fixed $\mathbf{c}$, we call $\{\mathbf{F} = \mathbf{c}\}$ a torus because this map provides a parameterization from $\{\mathbf{F} = \mathbf{c}\}$ to $\mathbb{R}^n/2\pi\mathbb{Z}^n \times \{\mathbf{c}\}$.

In this way Theorem 8.8 gives us a good understanding of the motion, but it is not complete. In particular, we are making no claim about what the fixed points look like (cf. the double well potential of Example 2.17).

Proof. As $\nabla F_1, \dots, \nabla F_n$ are linearly independent, there exists some $\delta > 0$ so that for $|\mathbf{c} - \mathbf{c}_0| < \delta$ the equations $\mathbf{F} = \mathbf{c}$ define smooth surfaces near $\mathbf{F} = \mathbf{c}_0$. For each $\mathbf{c}$ we pick a smoothly varying base point $x_0(\mathbf{c}) \in \{\mathbf{F} = \mathbf{c}\}$, and define the smooth map

$$\begin{array}{ccc} \mathbb{R}^n \times B_\delta(\mathbf{c}_0) & \to & \mathbb{R}^{2n} \\ (\mathbf{t}, \mathbf{c}) & \mapsto & e^{t_1 J \nabla F_1} \cdots e^{t_n \nabla F_n} x_0(\mathbf{c}) \end{array}$$

which flows out from the base point $x_0(\mathbf{c})$ within $\{\mathbf{F} = \mathbf{c}\}$ along the commuting flows $\dot{x} = J\nabla F_j(x)$.

As $\nabla F_1, \dots, \nabla F_n$ are linearly independent, this map is a local diffeomorphism. In fact, we claim that for fixed $\mathbf{c}$ this forms a covering map from $\mathbb{R}^n$ onto $\{\mathbf{F} = \mathbf{c}\}$. It only remains to show surjectivity, for which we use connectedness. Consider the set of points in $\{\mathbf{F} = \mathbf{c}\}$ accessible by this map. It is relatively open as the map is a local diffeomorphism. Its complement must then also be open, by the same argument for a different choice of base point. Therefore, as $\{\mathbf{F} = \mathbf{c}\}$ is connected then this set must contain the whole set.

For each $\mathbf{c}$, let L denote the set of times $\mathbf{t} \in \mathbb{R}^n$ for which the flow $e^{t_1 J \nabla F_1} \cdots e^{t_n \nabla F_n} x_0(\mathbf{c})$ returns to the base point $x_0(\mathbf{c})$. As the F_j flows commute, this set L is an additive subgroup of $\mathbb{R}^n$. This subgroup must be discrete, since the map is locally injective in a neighborhood of $x_0(\mathbf{c})$. Therefore L is a lattice. It is a fact that any such lattice must be of the form $\{\sum m_i e_i : m \in \mathbb{Z}^d\}$ for some generators $\{e_i\}_{i=1}^d \subset \mathbb{R}^n$ and $d \le n$. (To show this, we can pick e_1 closest to the origin, show that taking the quotient by e_1 yields a lattice with the same properties, and then induct.) Moreover, we must have a full set $d = n$ of generators because $\{\mathbf{F} = \mathbf{c}\}$ is compact. (Indeed, if we had $d < n$, then the image of our map would be a cylinder which is not compact.)

So far, we have a smooth map foliating the manifolds $\{\mathbf{F} = \mathbf{c} : |\mathbf{c} - \mathbf{c}_0| < \delta\}$ given by the coordinates $(\mathbf{t}, \mathbf{F})$, and we have a lattice $L(\mathbf{c}) \subset \mathbb{R}^n$ of full rank that depends smoothly on $\mathbf{c}$. By applying an invertible matrix $A(\mathbf{c})$ that smoothly varies with $\mathbf{c}$, we can find new coordinates $(\boldsymbol{\theta}, \mathbf{F})$ so that $L = \mathbb{Z}^n$:

$$\boldsymbol{\theta} \in \mathbb{R}^n/\mathbb{Z}^n, \qquad \boldsymbol{\theta} = A(\mathbf{F})\mathbf{t}.$$

However, these coordinates do not retain much of the Poisson structure; we have

$$\{F_i, F_j\} = 0, \qquad \{\theta_i, F_j\} = c_{ij}(\mathbf{F}), \qquad \{\theta_i, \theta_j\} = b_{ij},$$

where $c_{ij}(\mathbf{F})$ is an invertible matrix (since A is), and the b_{ij} are smooth functions that are otherwise unknown.

By the Jacobi identity, we have

$$\{b_{ij}, F_k\} + \{\{F_k, \theta_i\}, \theta_j\} + \{\{\theta_j, F_k\}, \theta_i\} = 0.$$

Note that $\{F_k, \theta_i\}$ and $\{\theta_j, F_k\}$ are only functions of $\mathbf{F}$ and not $\boldsymbol{\theta}$. Therefore, we deduce that $\{b_{ij}, F_k\}$ depends only on $\mathbf{F}$. On the other hand, we have

$$\{b_{ij}, F_k\} = \sum_{\ell=1}^{n} \left[\frac{\partial b_{ij}}{\partial \theta_\ell} \{\theta_\ell, F_k\} + \frac{\partial b_{ij}}{\partial F_\ell} \{F_\ell, F_k\} \right].$$

The second bracket $\{F_\ell, F_k\}$ above vanishes, while the first bracket $\{\theta_\ell, F_k\} = c_{ij}(\mathbf{F})$ is invertible and depends only on $\mathbf{F}$. Together, we conclude that $\frac{\partial b_{ij}}{\partial \theta_\ell}$ depends only on $\mathbf{F}$. (In other words, the gradient of b_{ij} within $\{\mathbf{F} = \mathbf{c}\}$ is constant.) Therefore, each b_{ij} also depends only on $\mathbf{F}$:

$$\{\theta_i, \theta_j\} = b_{ij}(\mathbf{F}), \tag{8.29}$$

since otherwise one of the $\frac{\partial b_{ij}}{\partial \theta_\ell}$ would have to depend on $\frac{\partial b_{ij}}{\partial \theta_\ell}$. (To verify this, we can expand $b_{ij}(\mathbf{F}, \boldsymbol{\theta})$ in a Fourier series in $\boldsymbol{\theta}$ with $\mathbf{F}$-dependent coefficients and use that the derivatives $\frac{\partial b_{ij}}{\partial \theta_\ell}$ are constant in $\boldsymbol{\theta}$.)

Lastly, we will perform one further changes of variables

$$\mathbf{I} = \mathbf{I}(\mathbf{F}), \qquad \boldsymbol{\phi} = \boldsymbol{\theta} + \mathbf{f}(\mathbf{I}) \tag{8.30}$$

to fix the Poisson bracket relations. We would like to make

$$\delta_{ij} = \{\theta_i, I_j\} = \sum_{k=1}^{n} \frac{\partial I_j}{\partial F_k} \{\theta_i, F_k\}. \tag{8.31}$$

The brackets $\{\theta_i, F_k\} = c_{ik}(\mathbf{F})$ are invertible, and so this uniquely prescribes the derivatives $\frac{\partial I_j}{\partial F_k}$. Moreover, we see that $\frac{\partial I_j}{\partial F_k}$ is invertible, and so $\mathbf{F} \mapsto \mathbf{I}$ will be a local diffeomorphism by the inverse function theorem, once we know it exists. The values of $\frac{\partial I_j}{\partial F_k}$ will correspond to the derivatives of a function $\mathbf{I}$ if

we have equality of mixed partials. To avoid the mess of directly applying $\frac{\partial}{\partial F_k}$ to $(c_{ij})^{-1}$, we instead take the bracket of (8.31) with θ_ℓ:

$$0 = \sum_{k=1}^{n} \frac{\partial I_j}{\partial F_k} \{\{\theta_i, F_k\}, \theta_\ell\} + \sum_{k,m=1}^{n} \frac{\partial^2 I_j}{\partial F_m \partial F_k} \{\theta_i, F_k\}\{F_m, \theta_\ell\}.$$

We want this expression to force the term $\frac{\partial^2 I_j}{\partial F_m \partial F_k}$ to be symmetric in k, m. The brackets $\{\theta_i, F_k\} = c_{ik}$ and $\{F_m, \theta_\ell\} = -c_{\ell m}$ are invertible, and multiplying by their inverses $c^{i\mu}$ and $-c^{m\nu}$ yields

$$\frac{\partial^2 I_j}{\partial F_\nu \partial F_\mu} = \sum_{i,k,m} \frac{\partial I_j}{\partial F_k} \{\{\theta_i, F_k\}, \theta_\ell\} c^{i\mu} c^{m\nu}. \tag{8.32}$$

Note that the Jacobi identity and (8.29) imply

$$\{\{\theta_i, F_k\}, \theta_\ell\} = \{\{\theta_\ell, F_k\}, \theta_i\}.$$

Together, we see that RHS(8.32) is indeed symmetric in μ and ν, and so the change of variables $\mathbf{I}(\mathbf{F})$ exists so that the bracket relations (8.31) hold.

It only remains to pick the function $\mathbf{f}$ in our change of variables (8.30). Currently, the variables $(\boldsymbol{\theta}, \mathbf{I})$ obey

$$\{\theta_i, I_j\} = \delta_{ij}, \qquad \{I_i, I_j\} = 0, \qquad \{\theta_i, \theta_j\} = \widetilde{b}_{ij}(\mathbf{I}). \tag{8.33}$$

The first relation is by our requirement (8.31), and the second relation is because $\mathbf{I} = \mathbf{I}(\mathbf{F})$. We want to choose $\mathbf{f}$ so that the change of variables $\boldsymbol{\phi} = \boldsymbol{\theta} + \mathbf{f}(\mathbf{I})$ makes

$$0 = \{\phi_i, \phi_j\} = \widetilde{b}_{ij}(\mathbf{I}) + \frac{\partial f_j}{\partial I_i}(\mathbf{I}) - \frac{\partial f_i}{\partial I_j}.$$

This prescribes the "curl" of $\mathbf{f}(\mathbf{I})$, and it is solvable by some $\mathbf{f}$ because

$$\widetilde{b}_{ij} = -\widetilde{b}_{ji}$$

by the antisymmetry of the bracket of θ_i, θ_j, and

$$\frac{\partial \widetilde{b}_{ij}}{\partial I_k} + \frac{\partial \widetilde{b}_{jk}}{\partial I_i} + \frac{\partial \widetilde{b}_{ki}}{\partial I_j} = 0$$

by the Jacobi identity for $\theta_i, \theta_j, \theta_k$.

Altogether, we have found a change of variables (8.30) which makes

$$\{\phi_i, I_j\} = \delta_{ij}, \qquad \{I_i, I_j\} = 0, \qquad \{\phi_i, \phi_j\} = 0.$$

Indeed, the first relation follows from the corresponding relation (8.33) for θ_i and that $\mathbf{f}$ is a function of $\mathbf{I}$. These are exactly the canonical relations (8.26) and (8.28), and so this concludes the proof of Theorem 8.8. □

8.6. Toda lattice

To conclude this chapter, we will present an introduction to an example of an infinite-dimensional completely integrable system. Define the one-dimensional potential

$$V(x) = e^{-x} - 1 + x, \tag{8.34}$$

and consider the following infinite chain of oscillators:

$$H = \sum_{i \in \mathbb{Z}} \tfrac{1}{2} p_i^2 + V(q_{i+1} - q_i). \tag{8.35}$$

This is a model for a one-dimensional crystal for the specific choice (8.34) of interaction potential. There is no issue in working with this infinite-dimensional system. Indeed, local well-posedness follows from the Picard–Lindelöf theorem in Banach spaces (Theorem A.2). As $V \geq 0$, we see that H controls the ℓ^2 norm of $\dot{q}$, and so conservation of energy implies global-in-time existence of solutions for localized excitations.

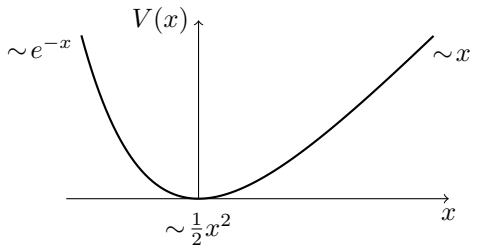


Figure 8.1: The potential energy (8.34).

The equations of motion are

$$\dot{q}_i = p_i, \qquad \dot{p}_i = -V'(q_i - q_{i-1}) + V'(q_{i+1} - q_i) = e^{q_{i-1}-q_i} - e^{-q_{i+1}+q_i} \tag{8.36}$$

for $i \in \mathbb{Z}$. Note that the contributions from the x term in (8.34) cancel out because q_i appears in the Hamiltonian for the ith and $(i-1)$st particles. As we will see, the infinite-dimensional system (8.36) turns out to be completely integrable in a certain sense. In order to demonstrate this however, we will need to exhibit *infinitely many* conserved quantities. To this end, we will need to move beyond physical quantities like momentum and energy, and develop a systematic tool that generates these conservation laws.

Our first step is the following (non-canonical) change of variables due to Flaschka:

$$b_i = -\tfrac{1}{2} p_i, \qquad a_i = \tfrac{1}{2} e^{(q_i - q_{i+1})/2}.$$

Note that a_i, b_i do not determine p_i, q_i exactly, but rather up to a global translation in q_i. This is okay by the conservation of total momentum. In terms of

the new variables a_i, b_i, our system (8.36) becomes

$$\dot{a}_i = (b_{i+1} - b_i)a_i, \qquad \dot{b}_i = 2(a_i^2 - a_{i-1}^2).$$

A straightforward computation shows that this system is equivalent to the matrix equation

$$\dot{L} = [P, L] = PL - LP \tag{8.37}$$

for the matrices

$$L(t) = \begin{pmatrix} \ddots & \ddots & & & \\ \ddots & b_0 & a_0 & & \\ & a_0 & b_1 & a_1 & \\ & & a_1 & b_2 & \ddots \\ & & & \ddots & \ddots \end{pmatrix}, \qquad P(t) = \begin{pmatrix} \ddots & \ddots & & & \\ \ddots & 0 & a_0 & & \\ & -a_0 & 0 & a_1 & \\ & & -a_1 & 0 & \ddots \\ & & & \ddots & \ddots \end{pmatrix}.$$

Together, L and P form what is called a **Lax pair** for the Toda lattice: the equations of motion can be recast as the equation (8.37) for L symmetric and P antisymmetric. So far, we intentionally are not making any rigorous claim about the existence of the matrices L, P. Nevertheless, each entry of the equation (8.37) only involves finitely many entries of L, P and thus makes sense.

The choice of Lax pair is certainly not unique; indeed, we are free to add any antisymmetric function of L to P without changing the RHS of (8.37). However, the structure of P is not surprising once we choose L to be tridiagonal: for example, we need the super-super-diagonal of $\dot{L}$ to vanish, which dictates the entries of P.

Formally, the existence of a Lax pair for a system implies that the system is completely integrable. If we let $U(t)$ denote the solution to

$$\dot{U} = PU, \qquad U(0) = I,$$

then we see that

$$L(t) = U(t)L(0)U^{-1}(t) \tag{8.38}$$

solves (8.37). Moreover, the matrix $U(t)$ remains orthogonal for all time since

$$\frac{\mathrm{d}}{\mathrm{d}t} U^T U = U^T P^T U + U^T P U = 0.$$

Therefore, the formula (8.38) for the solution tells us that $L(t)$ is orthogonally conjugate to its initial value. As conjugation preserves spectral information (e.g. it does not change the Jordan normal form), this implies that the eigenvalues of $L(t)$ are conserved.

In order to make this rigorous, we will restrict to finite dimensional subspaces of arbitrary size. We will impose that our solutions are periodic with period n:

$$q_{i+n} = q_i, \qquad p_{i+n} = p_i \quad \text{for all } i.$$

This periodicity is preserved by the dynamics. Now, the matrix equation (8.37) holds for the $n \times n$ matrices

$$L = \begin{pmatrix} b_1 & a_1 & & & a_n \\ a_1 & b_2 & a_2 & & \\ & a_2 & b_3 & \ddots & \\ & & \ddots & \ddots & a_{n-1} \\ a_n & & & a_{n-1} & b_n \end{pmatrix}, \qquad P = \begin{pmatrix} 0 & a_1 & & & -a_n \\ -a_1 & 0 & a_2 & & \\ & -a_2 & 0 & \ddots & \\ & & \ddots & \ddots & a_{n-1} \\ a_n & & & -a_{n-1} & 0 \end{pmatrix}$$

with $a_n = \frac{1}{2} e^{(q_n - q_1)/2}$.

For these finite-dimensional matrices, we are justified to compute their spectral properties. First, we note that the trace of L,

$$\operatorname{tr}(L) = \sum_{i=1}^{n} b_i = -\tfrac{1}{2} \sum_{i=1}^{n} p_i \tag{8.39}$$

is proportional to the total momentum. Moreover, we have

$$\begin{aligned} \operatorname{tr}\big(L^2\big) &= \sum_{i,j=1}^{n} L_{ij}^2 = \sum_{i,j=1}^{n} (b_i^2 + 2a_i^2) = \tfrac{1}{2} \sum_{i=1}^{n} \big\{ \tfrac{1}{2} p_i^2 + e^{q_{i+1} - q_i} \big\} \\ &= \tfrac{1}{2} H + \tfrac{1}{2} \sum_{i=1}^{n} \big\{ 1 - (q_{i+1} - q_i) \big\} = \tfrac{1}{2} H + \tfrac{1}{2} n, \end{aligned} \tag{8.40}$$

where H is the Hamiltonian (8.35) (with the summation only over one period $i = 1, \dots, n$), and in the last equality we noted that the sum of $q_{i+1} - q_i$ is telescoping and vanishes.

We know that both of the quantities (8.39) and (8.40) are conserved. In fact, for any $k \geq 1$ we have

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \operatorname{tr}\big(L^k\big) &= \operatorname{tr}\big(\dot{L} L^{k-1}\big) + \operatorname{tr}\big(L \dot{L} L^{k-2}\big) + \cdots + \operatorname{tr}\big(L^{k-1} \dot{L}\big) \\ &= \operatorname{tr}\big([P, L] L^{k-1}\big) + \operatorname{tr}\big(L [P, L] L^{k-2}\big) + \cdots + \operatorname{tr}\big(L^{k-1} [P, L]\big) \end{aligned}$$

Expanding $[P, L] = PL - LP$, we see that this sum is telescoping and we are left with

$$= \operatorname{tr}\{[P, L^k]\} = \operatorname{tr}\big(P L^k\big) - \operatorname{tr}\big(L^k P\big) = 0$$

by cycling the trace (which is justified for L finite-dimensional).

More generally, for any function $f(L)$ of the self-adjoint matrix L (which makes sense by the spectral theorem), we have

$$\frac{\mathrm{d}}{\mathrm{d}t} \operatorname{tr}\{f(L)\} = \operatorname{tr}\big\{[P, f(L)]\big\} = 0.$$

In particular,

$$\frac{\mathrm{d}}{\mathrm{d}t} \operatorname{tr}\big\{(L - z)^{-1}\big\} = 0.$$

The function $z \mapsto \operatorname{tr}\{(L-z)^{-1}\}$ is meromorphic with poles at the eigenvalues of L. From this, we deduce that the n eigenvalues of L are conserved. (This argument is not the most direct argument for finite-dimensional systems, but it has the advantage that it can be extended to infinite-dimensional operators.)

It follows that the system is completely integrable. So far, we have found n conserved quantities, namely the eigenvalues of L. A rather delicate computation then shows that these n quantities are also in involution; see [MZ05, §3.4] for details.

Next, we turn to the eigenvectors of L. Given

$$\psi(0) \in \mathbb{R}^n \smallsetminus \{0\} \quad \text{such that} \quad (L(0)-\lambda)\psi(0) = 0,$$

let $\psi(t)$ to be the solution to

$$\dot{\psi} = P\psi. \tag{8.41}$$

This is a Lipschitz ODE, and thus has a global solution $\psi(t)$ by the Picard–Lindelöf theorem (Theorem A.2). Then ψ obeys

$$\frac{\mathrm{d}}{\mathrm{d}t}(L(t)-\lambda)\psi(t) = [P,L]\psi - \lambda P\psi = P(L-\lambda)\psi.$$

By Grönwall's inequality (Lemma A.3), it follows that ψ remains an eigenvector for all $t \in \mathbb{R}$:

$$(L(t)-\lambda)\psi(t) \equiv 0.$$

(This computation is for real ψ; over the field $\mathbb{C}$, we can multiply by $e^{i\theta}$ and account for degenerate eigenvalues as well.) Moreover, the length of ψ is constant:

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi|^2 = P\psi\cdot\psi + \psi\cdot P\psi = \psi\cdot(P+P^T)\psi = 0.$$

Altogether, we conclude that the dynamics preserve the eigenvalues of L while the eigenvectors move around. With these eigenvectors in hand, we can construct the solution (8.38) for $L(t)$ to the equation (8.37).

So far, we have seen that the infinite-dimensional system (8.35) is completely integrable, in the sense that it is the limit of n-dimensional completely integrable systems as $n \to \infty$. For the remainder of this section, we will examine the corresponding action-angle coordinates. For this, it turns out to be more convenient to work with a different system corresponding to the matrices

$$L = \begin{pmatrix} b_1 & a_1 & & & \\ a_1 & b_2 & a_2 & & \\ & a_2 & b_3 & \ddots & \\ & & \ddots & \ddots & a_{n-1} \\ & & & a_{n-1} & b_n \end{pmatrix}, \qquad P = \begin{pmatrix} 0 & a_1 & & & \\ -a_1 & 0 & a_2 & & \\ & -a_2 & 0 & \ddots & \\ & & \ddots & \ddots & a_{n-1} \\ & & & -a_{n-1} & 0 \end{pmatrix}.$$

We have deleted the a_n entries in the corners of the matrix. This yields different finite-dimensional systems, but they correspond to the same Lax pair as $n \to \infty$. These a_n entries had originated from the x term in (8.34), and thus these

matrices are the Lax pair for the Hamiltonian (8.35) but with the new potential energy

$$V(x) = e^{-x}.$$

Note that this potential no longer has an equilibrium at $x = 0$.

Our action-angle coordinates will be closely related to the spectral properties of the operator L. The matrices L, P are now tridiagonal, and L is the operator for a discrete Sturm–Liouville problem. Consequently, we expect that L should have similar properties to a Sturm–Liouville operator. In particular, we claim that L has simple eigenvalues. If $Lu = \lambda u$ for some $u \in \mathbb{R}^n$, then the first entry reads

$$b_1 u_1 + a_1 u_2 = \lambda u_1.$$

As $a_j > 0$, we see that u_1 determines u_2. With these in hand, we then see that the second entry of $Lu = \lambda u$ determines u_3, and so on. In this way, u_1 uniquely determines the eigenvector u.

By the spectral theorem, we may construct the discrete probability measure

$$\mathrm{d}\mu(\lambda) = \sum_{j=1}^{n} \mu_j \delta(\lambda - \lambda_j)\,\mathrm{d}\lambda \quad \text{with} \quad \mu_j = u_{1j}^2.$$

Here, $(u_{1j}, \dots, u_{nj})$ is the eigenvector for the eigenvalue λ_j:

$$\sum_{\ell=1}^{n} L_{k\ell} u_{\ell j} = \lambda_j u_{kj}.$$

This makes

$$\langle e_1, f(L) e_1 \rangle = \int f(\lambda)\,\mathrm{d}\mu(\lambda)$$

for all $f : \mathbb{R} \to \mathbb{R}$. As we have just seen, L determines the measure μ. Conversely, given μ, we can reconstruct L as the matrix representation of the operation $f(\lambda) \mapsto \lambda f(\lambda)$ in $L^2(\mathrm{d}\mu)$ in the basis of orthonormal polynomials (i.e. the result of the Gram–Schmidt procedure applied to $1, x, x^2, \dots, x^{n-1}$). In other words, the three middle entries of the kth row of L must satisfy

$$\lambda p_k(\lambda) = a_k p_{k+1}(\lambda) + b_k p_k(\lambda) + a_{k-1} p_{k-1}(\lambda).$$

We know that the other entries must be zero, because the RHS must have degree $k + 1$ and we have the orthogonality condition

$$\int \lambda p_k(\lambda)\, p_{k-2}(\lambda)\,\mathrm{d}\lambda = \int p_k(\lambda)\, \lambda p_{k-2}(\lambda)\,\mathrm{d}\lambda = 0$$

since λp_{k-2} has degree $k - 1$.

Next, we turn to the evolution of μ. We have already seen that the eigenvalues λ_j of L are conserved:

$$\dot{\lambda}_j = 0,$$

and that the eigenvectors u evolve according to (8.41). (We proved this for our previous Lax pair, but the proof only relied on the evolution equation (8.37) and thus still applies.) Consequently, the evolution of the weights μ_j is

$$\begin{aligned}\dot{\mu}_j &= 2u_{1j}\dot{u}_{1j} = 2u_{1j}a_1u_{2j} = 2(\lambda_j - b_1)u_{1j}^2 \\ &= 2(\lambda_j - b_1)\mu_j = 2\biggl(\sum_{k=1}^{n}(\lambda_j - \lambda_k)\mu_k\biggr)\mu_j,\end{aligned}$$

where in the last equality we used

$$b_1 = \langle e_1, Le_1\rangle = \int \lambda \,\mathrm{d}\lambda = \sum_{k=1}^{n} \lambda_k\mu_k.$$

The solution is given by

$$\mu_j(t) = \frac{e^{2\lambda_j t}\mu_j(0)}{\sum e^{2\lambda_k t}\mu_k(0)}. \tag{8.42}$$

This is an exponential with rate $2\lambda_j$ that is normalized so that μ is a probability measure. Together, the eigenvalues λ_j and the weights μ_j provide a complete and simple description of the flow. The eigenvalues are action variables, as they are conserved and in involution. Strictly speaking, the weights μ_j are not angle variables since they evolve exponentially rather than linearly; this is easily remedied by taking their logarithm, but this is not strictly necessary as the μ_j already provide an equally simple description of the motion. Altogether, the transformation from a_j, b_j to λ_j, μ_j is like a nonlinear version of the Fourier transform: just like the Fourier transform linearizes a linear constant-coefficient differential equation, we have found a change of coordinates λ_j, μ_j which linearizes the flow.

It remains to invert our transformation and recover a_j, b_j from λ_j, μ_j. Let

$$c_j = \int x^j \,\mathrm{d}\mu,$$

and consider the $k \times k$ Hankel determinant of the c_j:

$$h_k = \det \begin{pmatrix} c_0 & c_1 & \cdots & c_{k-1} \\ c_1 & c_2 & \cdots & c_k \\ \vdots & \vdots & \ddots & \vdots \\ c_{k-1} & c_k & \cdots & c_{2k-2} \end{pmatrix}.$$

These quantities are closely related to the Gram–Schmidt procedure that produces the polynomials $p_k(x)$. Specifically, we have

$$p_k(x) \propto \det \begin{pmatrix} c_0 & c_1 & \cdots & c_k \\ c_1 & c_2 & \cdots & c_{k+1} \\ \vdots & \vdots & \ddots & \vdots \\ c_{k-1} & c_k & \cdots & c_{2k-1} \\ 1 & x & \cdots & x^k \end{pmatrix}. \tag{8.43}$$

This is because the RHS is a polynomial of degree k, and the Andréief–Heine identity

$$\int x^\ell \,\mathrm{RHS}(8.43)\,\mathrm{d}x = \det\begin{pmatrix} c_0 & c_1 & \cdots & c_k \\ c_1 & c_2 & \cdots & c_{k+1} \\ \vdots & \vdots & \ddots & \vdots \\ c_{k-1} & c_k & \cdots & c_{2k-1} \\ c_\ell & c_{\ell+1} & \cdots & c_{\ell+k} \end{pmatrix}$$

implies that the integral vanishes for $\ell \le k-1$ (as required by the Gram–Schmidt procedure). It turns out that the Hankel determinants of the c_j also allow us to recover the a_k via the formula

$$a_k = \sqrt{\frac{h_{k-1}h_{k+1}}{h_k^2}}.$$

The change of variables from the λ_j, μ_j back to the a_j, b_j is called the **inverse scattering transformation**. (The reason for this name is that it is common for infinite-dimensional completely integrable systems for the action-angle variables to be connected to scattering theory, and inverting the change of variables requires new work.)

Finally, we note that the simple evolution of λ_j, μ_j also provides a description of the long-time behavior. After reordering $\lambda_1 > \lambda_2 > \cdots > \lambda_n$, we see that the exponential $e^{2\lambda_1 t}$ is the dominant term as $t \to \infty$, and so from the explicit solutions (8.42) we have

$$\mathrm{d}\mu \to \delta(\lambda - \lambda_1)\,\mathrm{d}\lambda \quad \text{as } t \to \infty.$$

Therefore

$$b_1 = \int \lambda\,\mathrm{d}\lambda \to \lambda_1, \qquad a_1 \to 0,$$

and so

$$L \to \begin{pmatrix} \lambda_1 & 0 & & & \\ 0 & * & * & & \\ & * & * & \ddots & \\ & & \ddots & \ddots & * \\ & & & * & * \end{pmatrix}.$$

This resembles the first step of the QR algorithm for the symmetric tridiagonal matrix L. In fact, we can obtain a dynamical version of the full QR algorithm by removing the first row and column of L and repeating the process. Indeed, the next order exponential is $e^{2\lambda_2 t}$ which yields

$$\mathrm{d}\mu = Z^{-1}\big\{\delta(\lambda-\lambda_1) + e^{-2(\lambda_1-\lambda_2)t}\delta(\lambda-\lambda_2) + \mathcal{O}\big(e^{-2(\lambda_1-\lambda_3)t}\big)\big\}\,\mathrm{d}\lambda$$

for Z a normalization constant, and this suggests $b_2 \to \lambda_2$ and $a_2 \to 0$. This can be made rigorous by evaluating the λ_j in terms of Hankel determinants as $t \to \infty$; see [MZ05, §3.4] for details.

8.7. Exercises

8.1 (Example of Birkhoff normal form)**.** Fix $\omega > 0$ and $a \in \mathbb{R}$, and consider the Hamiltonian

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}\omega^2 q^2 + aq^4.$$

(a) Compute the Birkhoff normal form up to degree 4.

(b) Provide a correspondingly accurate approximation for the period of oscillation as a function of energy.

8.2 (Example of Liouville integration)**.** Fix $\omega > 0$ and $a \in \mathbb{R}$, and consider the Hamiltonian

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}\omega^2 q^2 + aq^4.$$

(a) Using conservation of energy under the above Hamiltonian flow, show that the dynamics yield

$$\dot{q} = f(E, q)$$

for suitable explicit function(s) f.

(b) This equation is separable. Thus one can formally solve for $p(t)$ and $q(t)$ via integration. Use this method to derive a formula for the period of oscillation (as a function of energy) in the form of a definite integral.

8.3 (Harmonic oscillator)**.** The one-dimensional harmonic oscillator has Hamiltonian

$$H = T + V = \tfrac{1}{2m}p^2 + \tfrac{m}{2}\omega^2 x^2.$$

(a) Find the angle variable I and show that the energy as a function of the angle variable I is $h(I) = \omega I$.

(b) Write down (but do not evaluate) the integral for the generating function Φ, and show that the angle variable is given by

$$\phi = \tan^{-1}\left(\frac{x}{\sqrt{\frac{2I}{m\omega} - x^2}}\right) + \text{constant}.$$

(c) Using the linear evolution of ϕ, find the solution $x(t)$ for the motion.

CHAPTER 9

SYMPLECTIC GEOMETRY

Symplectic geometry is the differential geometric generalization of the time-independent Hamiltonian structure of phase space to general manifolds, and the physical results for conservative systems from the previous chapter can be lifted to this perspective. The material for this section is based on [Arn89, Ch. 8] and [Lee13, Ch. 22].

9.1. Symplectic structure

Let M be a smooth even-dimensional manifold of dimension $2n$. A **symplectic form** or **symplectic structure** on M is a two-form ω on M that is closed ($\mathrm{d}\omega = 0$) and **nondegenerate**: for each $x \in M$ the map $T_xM \to T_x^*M$ which takes $\xi \mapsto \xi \lrcorner \omega = \omega(\xi, \cdot)$ is invertible. The pair (M, ω) is called a **symplectic manifold**. There are other more easily verifiable criteria for a two-form ω (cf. Exercise 9.1), but conceptually this is the classification we will rely upon. Heuristically, the symplectic form ω is an identification of the tangent and cotangent spaces at each point in M, which bears resemblance to Riemannian structure but as we shall see exhibits drastically different behavior.

Symplectic structures are equivalent to nondegenerate Poisson structures via inverting the structure matrix J:

Example 9.1. If is the structure matrix of a canonical Poisson bracket

$$\{\cdot, \cdot\} = \sum_{i,j=1}^{n} J^{ij}(x) \frac{\partial}{\partial x^i} \otimes \frac{\partial}{\partial x^j}$$

as in Corollary 7.9, then

$$\omega = \sum_{i,j=1}^{n} J_{ij}(x)\, \mathrm{d}x^i \otimes \mathrm{d}x^j \tag{9.1}$$

is a symplectic form, where J_{ij} are the entries of the inverse of the matrix J^{ij}.

This is the dual object to Poisson brackets. Indeed, so far we have been viewing a vector field X as an operator

$$X(f) = \sum_{i=1}^{n} X^i(x) \frac{\partial f}{\partial x^i}$$

on smooth functions f. We can also view this as the exterior derivative $\mathrm{d}f(X)$, where f operates on X and $\mathrm{d}x^i$ is defined by

$$\mathrm{d}x^i\left(\frac{\partial}{\partial x^j}\right) = \begin{cases} 1 & i = j, \\ 0 & i \neq j. \end{cases}$$

The operator (9.1) is an exterior 2-form because J is antisymmetric. It is also closed because J satisfies the Jacobi identity (Exercise 9.2).

In particular, if we take the canonical Poisson structure in the previous example, we obtain:

Example 9.2 (Canonical symplectic form)**.** Consider a cotangent bundle T^*N of an n-dimensional manifold N, or simply the Euclidean space $T^*\mathbb{R}^n = \mathbb{R}^n_q \times \mathbb{R}^n_p$. Then the two-form

$$\omega = \mathrm{d}p \wedge \mathrm{d}q = \sum_{i=1}^{n} \mathrm{d}p^i \wedge \mathrm{d}q^i \tag{9.2}$$

is a symplectic form on T^*N, and is called the **canonical symplectic form** on the cotangent bundle; we will later see how this form naturally encapsulates Hamilton's equations. This form is closed, since it is the exterior derivative of the one-form

$$p\,\mathrm{d}q = \sum_{i=1}^{n} p^i\,\mathrm{d}q^i, \tag{9.3}$$

which is in turn called the **tautological one-form** on T^*M; we first saw this form in the period integral (2.9) and then again later in defining the action variable (6.20). To see that ω is nondegenerate, fix $(q,p) \in T^*N$ and let $(v_1,\dots,v_n,a_1,\dots,a_n) \in T_{(q,p)}(T^*N)$ denote the dual basis to $(\mathrm{d}q,\mathrm{d}p)$ so that

$$\mathrm{d}q^i(v_j) = \delta_{ij}, \qquad \mathrm{d}p^i(a_j) = \delta_{ij}, \qquad \mathrm{d}q^i(a_j) = \mathrm{d}p^i(v_j) = 0$$

for $i,j = 1,\dots,n$. Often in differential topology we write ∂_{q_i} for the dual vector to $\mathrm{d}q^i$, but physically we like to think of the tangent vector to a point in phase space as the velocity and (mass-times-)acceleration. The action of ω on these basis vectors is

$$\omega(v_i,v_j) = \omega(a_i,a_j) = 0, \qquad \omega(v_i,a_j) = -\omega(a_j,v_i) = \delta_{ij}$$

for $i,j = 1,\dots,n$. To check nondegeneracy, fix $\xi \in T_{(q,p)}(T^*N)$ and suppose we have $\omega(\xi,\eta) = 0$ for all $\eta \in T_{(q,p)}(T^*N)$. Expanding $\xi = \sum_{i=1}^{n}(b^i v_i + c^i a_i)$ for constants $b^i, c^i \in \mathbb{R}$, we see that

$$0 = \omega(\xi,v_i) = -c^i, \qquad 0 = \omega(\xi,a_i) = b^i$$

and so $\xi = 0$ as desired.

In fact, the form of Example 9.2 is the fundamental example in the following sense.

Theorem 9.3 (Darboux's theorem)**.** *Let (M, ω) be a $2n$-dimensional symplectic manifold. For any $\xi \in M$ there exists local coordinates (q, p) centered at ξ with respect to which ω has the representation* (9.2)*.*

This follows from Theorem 7.18, but also can be proved directly [Lee13, Th. 22.13].

Symplectic manifolds are automatically orientable because ω^n is a nonvanishing $2n$ form on M. Indeed, if we fix $x \in M$ and write $\omega = \sum_i \mathrm{d}p^i \wedge \mathrm{d}q^i$ at x, then the n-fold wedge product

$$\omega^n = \sum_I \mathrm{d}p^{i_1} \wedge \mathrm{d}q^{i_1} \wedge \cdots \wedge \mathrm{d}p^{i_d} \wedge \mathrm{d}q^{i_d}$$

where the sum ranges over all multi-indices $I = (i_1, \ldots, i_n)$ of length n. Any term where I contains a repeated index is zero because $\mathrm{d}q^i \wedge \mathrm{d}q^i = 0$, and since 2-forms commute under the wedge product then we can rewrite this as

$$\omega^d = d! \, \mathrm{d}p^1 \wedge \mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}p^d \wedge \mathrm{d}q^d.$$

This is nonvanishing at x by definition of the nondegeneracy of ω.

9.2. Hamiltonian vector fields

Next let us see how to use the symplectic structure to obtain the familiar dynamics from a Hamiltonian. Let (M, ω) be a symplectic manifold and $H : M \to \mathbb{R}$ be a smooth function. Then $\mathrm{d}H$ is a differential one-form which associates a covector to each point in M. On the other hand, for Hamilton's equations we need to specify a vector field for the right-hand side of the differential equation. By definition, for each $x \in M$ the map $T_xM \to T_x^*M$ which takes $\xi \mapsto \xi \lrcorner \omega$ is invertible, and so let $J : T_x^*M \to T_xM$ denote its inverse. Then $J\,\mathrm{d}H$ is a vector field on M, called the **Hamiltonian vector field** associated to the Hamiltonian H. The induced flow $e^{tJ\,\mathrm{d}H} : M \to M$, $x_0 \mapsto x(t)$ defined to solve the ODE

$$\dot{x}(t) = J\,\mathrm{d}H(x(t)), \qquad x(0) = x_0 \tag{9.4}$$

is called a **Hamiltonian flow** on M. In differential geometry the notation $\widehat{\omega} : T_xM \to T_x^*M$ is used for the map $\xi \mapsto \xi \lrcorner \omega$, and so in place of J the notations $\widehat{\omega}^{-1}$ and

$$X_H := \widehat{\omega}^{-1}(\mathrm{d}H) \qquad \Longleftrightarrow \qquad X_H \lrcorner \omega = \mathrm{d}H \tag{9.5}$$

are often used.

Example 9.4. Consider the canonical symplectic form (9.2) on the Euclidean phase space $T^*\mathbb{R}^n = \mathbb{R}^n_q \times \mathbb{R}^n_p$. On Euclidean space we already have a natural identification of vectors and covectors via the dot product, and we can express J as a linear transformation in terms of this identification. Given a vector field

$$X = \sum_{i=1}^n \left(b^i \frac{\partial}{\partial q^i} + c^i \frac{\partial}{\partial p^i} \right)$$

for some smooth coefficients b^i and c^i, we compute

$$X \lrcorner \omega = \sum_{i=1}^{n} \left(c^i \, \mathrm{d}q^i - b^i \, \mathrm{d}p^i \right) = \begin{pmatrix} c \\ -b \end{pmatrix} = J \begin{pmatrix} b \\ c \end{pmatrix}$$

and hence

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{9.6}$$

for I the identity matrix. Writing

$$\mathrm{d}H = \frac{\partial H}{\partial q} \, \mathrm{d}q + \frac{\partial H}{\partial p} \, \mathrm{d}p = \sum_{i=1}^{n} \left(\frac{\partial H}{\partial q^i} \, \mathrm{d}q^i + \frac{\partial H}{\partial p^i} \, \mathrm{d}p^i \right) = \begin{pmatrix} \frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial p} \end{pmatrix},$$

we have

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = J \, \mathrm{d}H = \begin{pmatrix} \frac{\partial H}{\partial p} \\ -\frac{\partial H}{\partial q} \end{pmatrix}$$

which agrees with Hamilton's equations (7.2).

Symplectic geometry is the generalization of time-independent Hamiltonian dynamics since the Hamiltonian function H is automatically conserved under its Hamiltonian flow.

Proposition 9.5 (Conservation of energy)**.** *Let (M, ω) be a symplectic manifold and let H be a smooth function on M. Then H is constant along the integral curves of $J \, \mathrm{d}H$, and when $\mathrm{d}H \neq 0$ the vector field $\mathrm{d}H$ is tangent to the level sets of H.*

Proof. Both are a consequence of

$$(J \, \mathrm{d}H)(H) = \mathrm{d}H(J \, \mathrm{d}H) = \omega(J \, \mathrm{d}H, J \, \mathrm{d}H) = 0,$$

which holds since ω is alternating. □

9.3. Integral invariants

Consider a smooth diffeomorphism $g : M \to M$. A k-form η is said to be an integral invariant for g if

$$\int_{g(N)} \eta = \int_N \eta \tag{9.7}$$

for all orientable k-dimensional submanifolds N with boundary.

Theorem 9.6. *A Hamiltonian flow $g_t = e^{tJ \, \mathrm{d}H}$ preserves the symplectic structure: $g_t^* \omega = \omega$. In other words, the symplectic form ω is an integral invariant of g_t.*

Proof. The map g_t is smoothly homotopic to the identity via the family of diffeomorphisms g_s, $s \in [0,t]$, in the sense that at time $s = 0$ the map $g_0 : M \to M$ is the identity, and at time $s = t$ the map $g_t : M \to M$ is what we are given. Fix N a smooth orientable 2-dimensional submanifold, and let $\Omega_N := \{g_s(N) : s \in [0,t]\}$ denote the image of N under the homotopy. We can think of ω_N as an orientable 3-manifold in $[0,t] \times M$ or as being immersed in M. With this choice of orientation we have

$$\partial\Omega_N = g_t(N) \cup (-N) \cup (-\Omega_{\partial N}). \tag{9.8}$$

We claim that for any smooth curve γ in M we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_\gamma} \omega = \int_{g^t(\gamma)} \mathrm{d}H, \tag{9.9}$$

where H is the Hamiltonian for the flow g^t. Let $\phi : [a,b] \to M$ be a parametrization of γ. Then Ω_γ is parameterized by $\Phi(s,x) := g^s(\phi(x))$ and we have

$$\int_{\Omega_\gamma} \omega = \int_0^t \int_a^b \omega\left(\frac{\partial\Phi}{\partial x}, \frac{\partial\Phi}{\partial s}\right) \mathrm{d}x\,\mathrm{d}s$$

where $\frac{\partial\Phi}{\partial s}(s,x)$ is in $T_{\Phi(s,x)}M$. By definition of the Hamiltonian phase flow $g_t = e^{tJ\,\mathrm{d}H}$ the tangent vector $\frac{\partial\Phi}{\partial s}$ points in the direction of $J\,\mathrm{d}H$, and so we have $\omega(\frac{\partial\Phi}{\partial x}, \frac{\partial\Phi}{\partial s}) = \mathrm{d}H(\frac{\partial\Phi}{\partial x})$. Therefore

$$\int_{\Omega_\gamma} \omega = \int_0^t \int_a^b \mathrm{d}H\left(\frac{\partial\Phi}{\partial x}\right) \mathrm{d}x\,\mathrm{d}s = \int_0^t \left(\int_{g^s(\gamma)} \mathrm{d}H\right) \mathrm{d}s,$$

and the identity (9.9) follows from the fundamental theorem of calculus.

For a closed curve like ∂N we note that

$$\int_{g^t(\partial N)} \mathrm{d}H = \int_{g^t(\emptyset)} H = 0,$$

and so the identity (9.9) implies

$$\int_{\Omega_{\partial N}} \omega = 0. \tag{9.10}$$

As ω is closed by definition, then by Stokes' theorem we have

$$0 = \int_{\Omega_N} \mathrm{d}\omega = \int_{\partial\Omega_N} \omega.$$

Decomposing the boundary $\partial\Omega_N$ according to (9.8) we obtain

$$0 = \int_{g_t(N)} \omega - \int_N \omega - \int_{\Omega_{\partial N}} \omega.$$

From (9.10) we know the last integral vanishes, and so we conclude that ω is an integral invariant of g_t. □

In the previous section we saw that ω^n defines a volume form on M and so we immediately obtain an analog of Theorem 7.25.

Corollary 9.7 (Liouville's theorem)**.** *Each of the forms ω^2, ω^4, ... is preserved by a Hamiltonian flow. In particular, every Hamiltonian flow preserves the volume form ω^n.*

In section 7.6 we defined a canonical transformation to be a change of coordinates that preserved the Poisson structure. Given a cotangent bundle $M = T^*Q$ with canonical symplectic form $\omega = \mathrm{d}p \wedge \mathrm{d}q$, we analogously define a (time-independent) canonical transformation to be a function $g : T^*Q \to T^*Q$ which satisfies

$$g^*(p\,\mathrm{d}q) = p\,\mathrm{d}q + \mathrm{d}S. \tag{9.11}$$

This definition does not make $p\,\mathrm{d}q$ an integral invariant for a canonical transformation, since the condition (9.7) only holds for closed curves N. Instead, we employ the following useful observation.

Proposition 9.8. *Let $g : M \to M$ be a smooth diffeomorphism. If η is a k-form such that* (9.7) *holds for only closed orientable k-submanifolds N, then $\mathrm{d}\eta$ is an integral invariant.*

Proof. Let N be an orientable $(k+1)$-submanifold. Then by Stokes' theorem we have

$$\int_N \mathrm{d}\eta = \int_{\partial N} \eta, \qquad \int_{g(N)} \mathrm{d}\eta = \int_{\partial g(N)} \eta = \int_{g(\partial N)} \eta.$$

As ∂N is closed then these two right-hand sides are equal by premise. Therefore we conclude that (9.7) holds for the form $\mathrm{d}\eta$, and hence $\mathrm{d}\eta$ is an integral invariant. □

Noting that $\mathrm{d}(p\,\mathrm{d}q) = \mathrm{d}p \wedge \mathrm{d}q$, we conclude:

Corollary 9.9. *Canonical transformations preserve the symplectic form ω and the volume form ω^n.*

In Euclidean phase space $T^*\mathbb{R}^n$, any Hamiltonian flow is automatically a canonical transformation. However, the converse of Proposition 9.8 is not true in general, and so Theorem 9.6 does not imply the identity (9.11). We must assume that M is simply connected in order for Hamiltonian flows to be canonical transformations, since then Theorem 9.6 implies (9.11).

9.4. Poisson bracket

In section 7.3 we saw how to phrase Hamiltonian dynamics in terms of the Poisson bracket, and in this section we will see how this notion manifests in terms of symplectic structure. For smooth functions $f, g \in C^\infty(M)$ on a symplectic manifold (M, ω) we define the **Poisson bracket** of f and g to be

$$\{f, g\} = \omega(J\,\mathrm{d}f, J\,\mathrm{d}g) = \mathrm{d}g(J\,\mathrm{d}f) = (J\,\mathrm{d}f)(g). \tag{9.12}$$

As in (7.9) the Poisson bracket $\{H, f\}$ is also the evolution of the quantity f under the Hamiltonian flow H, since the Lie derivative of the function f along $J\,\mathrm{d}H$ is given by

$$\mathcal{L}_{J\,\mathrm{d}H} f = \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0} f \circ e^{tJ\,\mathrm{d}H} = (J\,\mathrm{d}H)(f) = \{H, f\} \tag{9.13}$$

according to the definition (9.4) of the Hamiltonian flow. In particular, we again have that f is conserved by the Hamiltonian flow of H if and only if $\{H, f\} = 0$.

Example 9.10. Let us check that the new definition (9.12) agrees with the phase space definition (7.10) on Euclidean space $T^*\mathbb{R}^n = \mathbb{R}^n_q \times \mathbb{R}^n_p$. Using the calculation of J from Example 9.4 we have

$$J\,\mathrm{d}f = J\left(\frac{\partial f}{\partial q}\,\mathrm{d}q + \frac{\partial f}{\partial p}\,\mathrm{d}p\right) = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial f}{\partial q} \\ \frac{\partial f}{\partial p} \end{pmatrix} = \frac{\partial f}{\partial p}\frac{\partial}{\partial q} - \frac{\partial f}{\partial q}\frac{\partial}{\partial p}.$$

Consequently, the definition (9.12) yields

$$\{f, g\} = (J\,\mathrm{d}f)(g) = \frac{\partial f}{\partial p}\frac{\partial g}{\partial q} - \frac{\partial f}{\partial q}\frac{\partial g}{\partial p},$$

which agrees with the first definition (7.10).

The properties listed in section 7.3 resemble those of the commutator because the Poisson bracket at the level of functions corresponds to the commutator of the respective Hamiltonian vector fields.

Proposition 9.11. *If (M, ω) is a symplectic manifold, then the Poisson bracket is the Hamiltonian of the commutator of the corresponding Hamiltonian vector fields:*

$$J\,\mathrm{d}\{f, g\} = [J\,\mathrm{d}f, J\,\mathrm{d}g]. \tag{9.14}$$

In particular, the vector space $C^\infty(M)$ is a Lie algebra under the Poisson bracket: the Poisson is bilinear, antisymmetric, and satisfies the Jacobi identity.

Proof. In fact, it suffices to prove that the Poisson bracket satisfies the Jacobi identity

$$\{\{f, g\}, h\} + \{\{g, h\}, f\} + \{\{h, f\}, g\} = 0 \tag{9.15}$$

for arbitrary smooth functions $f, g, h \in C^\infty(M)$. This is sufficient because we can use the antisymmetry of ω to write

$$\{\{f, g\}, h\} = \{f, \{g, h\}\} - \{g, \{f, h\}\},$$

and recognizing the Poisson bracket as a Lie derivative via (9.13) we conclude

$$\mathcal{L}_{J\,\mathrm{d}\{f,g\}} h = \mathcal{L}_{J\,\mathrm{d}f}\mathcal{L}_{J\,\mathrm{d}g} h - \mathcal{L}_{J\,\mathrm{d}g}\mathcal{L}_{J\,\mathrm{d}f} h = \mathcal{L}_{[J\,\mathrm{d}f, J\,\mathrm{d}g]} h.$$

As $h \in C^\infty(M)$ is arbitrary, the identity (9.14) must hold.

It remains to demonstrate the Jacobi identity (9.15). The left-hand side of (9.15) is a combination of terms which each have at least one second order derivative. Isolating the terms containing second order derivatives of f and recognize the Poisson bracket as a Lie derivative via (9.13), we have

$$\begin{aligned}\{\{f,g\},h\}+\{\{h,f\},g\} &= \{h,\{g,f\}\}-\{g,\{h,f\}\}\\ &= \mathcal{L}_{J\,\mathrm{d}h}\mathcal{L}_{J\,\mathrm{d}g}f-\mathcal{L}_{J\,\mathrm{d}g}\mathcal{L}_{J\,\mathrm{d}h}f.\end{aligned}$$

However, we know $\mathcal{L}_{J\,\mathrm{d}h}\mathcal{L}_{J\,\mathrm{d}g}-\mathcal{L}_{J\,\mathrm{d}g}\mathcal{L}_{J\,\mathrm{d}h}=\mathcal{L}_{[J\,\mathrm{d}h,J\,\mathrm{d}g]}$ is only a first order differential operator, and so we conclude that the terms with second order derivatives of f vanish. Lastly, since the left-hand side of (9.15) is symmetric in f, g, and h, we conclude that there can be no second order derivatives and hence must vanish. □

9.5. Time-dependent systems

Hamilton's equations (7.2) remain valid for time-dependent Hamiltonian systems, and yet thus far we have only allowed H to be a smooth function on phase space M. This section is dedicated to extending the symplectic geometry developed thus far to time-dependent Hamiltonian systems.

Let (M,ω) be a $2n$-dimensional symplectic manifold, and define the **extended phase space** $M\times\mathbb{R}$. Given a possibly time-dependent Hamiltonian H, we define the **Poincaré–Cartan one-form** locally in terms of the canonical coordinates (q,p) on M guaranteed by Theorem 9.3 as

$$\tau = p\,\mathrm{d}q - H\,\mathrm{d}t = \sum_{i=1}^{n} p^i\,\mathrm{d}q^i - H\,\mathrm{d}t. \tag{9.16}$$

Note that the first term above is the tautological one-form $p\,\mathrm{d}q$ on M, the differential of which yields the symplectic form ω. This is the form that we insisted be preserved by a canonical transformation in (9.11), and the same notion of canonical transformations holds on a general extended phase space $M\times\mathbb{R}$ in terms of the canonical coordinates (q,p,t).

The extended phase space $M\times\mathbb{R}$ together with the Poincaré–Cartan one-form τ do indeed define a contact manifold, but as we will see in the next chapter it is not the natural contact extension of M since τ depends on the system's Hamiltonian H.

On $M\times\mathbb{R}$ we define the **extended Hamiltonian vector field**

$$Y_H = X_H + \frac{\partial}{\partial t}, \tag{9.17}$$

where $X_H(t)$ is the Hamiltonian vector field on $M\times\{t\}$ defined by (9.4). In analogy with the second condition of (9.5), the vector field (9.17) is the unique solution to

$$Y_H \lrcorner \mathrm{d}\tau = 0. \tag{9.18}$$

The flow of Y_H is given by

$$\dot{q}^i = \frac{\partial H}{\partial p^i}, \qquad \dot{p}^i = -\frac{\partial H}{\partial q^i}, \qquad \dot{t} = 1, \tag{9.19}$$

which is just Hamilton's equations (7.2) joined with the trivial equation $\dot{t} = 1$. It follows that any smooth time-dependent function f on $M \times \mathbb{R}$ evolves according to

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \{H, f\}_{p,q} + \frac{\partial f}{\partial t},$$

as was the case in section 7.3. In particular, a time-dependent Hamiltonian H is no longer conserved under its own flow.

Example 9.12. The authors of [Cal41, Kan48] showed that in addition to naturally occurring time-dependent Hamiltonian systems, this framework can also be applied to some systems which are time-independent and dissipative by introducing artificial time dependence into the Hamiltonian. Consider the one-dimensional Hamiltonian system

$$H(Q, P, t) := e^{-\gamma t}\frac{P^2}{2m} + e^{\gamma t}V(Q) \tag{9.20}$$

on the extended phase space $\mathbb{R}_Q \times \mathbb{R}_P \times \mathbb{R}_t$, where $\gamma \geq 0$ is a constant and the coordinates Q, P are related to the physical coordinates q, p by the non-canonical transformation

$$P = e^{\gamma t}p, \qquad Q = q.$$

Then the equations of motion (9.19) yield

$$m\ddot{q} + m\gamma\dot{q} + V'(q) = 0.$$

This represents a Newtonian system with a friction force that depends linearly on the velocity, like the damped harmonic oscillator of Example 2.9.

9.6. Locally Hamiltonian vector fields

In section 9.1 we called a vector field V on a symplectic manifold (M, ω) Hamiltonian if it is equal to $J\,\mathrm{d}H$ for some smooth function $H \in C^\infty(M)$, and in Theorem 9.6 we saw that ω is necessarily invariant under the flow of $J\,\mathrm{d}H$. In fact, any smooth vector field V on M whose flow leaves ω invariant (i.e. $(e^{tV})^*\omega = \omega$) is called **symplectic**. However, a vector field being Hamiltonian is a global condition—in the sense that the corresponding Hamiltonian H must extend smoothly to all of M—while being symplectic is a pointwise condition and is hence only local.

Consequently, a smooth vector field V on M is called **locally Hamiltonian** (as opposed to **globally** Hamiltonian) if for each point p there exists a neighborhood on which V is Hamiltonian. As an extension of Theorem 9.6, locally Hamiltonian vector fields are exactly those which are symplectic.

Proposition 9.13. *Let (M, ω) be a symplectic manifold. A smooth vector field V on M is symplectic if and only if it is locally Hamiltonian. If M is also simply connected, then every locally Hamiltonian vector field is globally Hamiltonian.*

Proof. Differentiating the condition $(e^{tV})^*\omega = \omega$ with respect to t at $t = 0$, we see that a vector field V is symplectic if and only if $\mathcal{L}_V\omega = 0$. From Cartan's magic formula we have

$$\mathcal{L}_V\omega = \mathrm{d}(V \lrcorner \omega) + V \lrcorner \mathrm{d}\omega = \mathrm{d}(V \lrcorner \omega)$$

since ω is closed. Therefore V is symplectic if and only if $V \lrcorner \omega$ is closed.

If V is locally Hamiltonian, then in a neighborhood of any point there exists a function f so that $V = J\,\mathrm{d}f$, and hence $V \lrcorner \omega = \mathrm{d}f$ which is certainly closed. Conversely, if V is a symplectic vector field, then $V \lrcorner \omega$ is closed and hence exact in a neighborhood of any point, and writing $V \lrcorner \omega = \mathrm{d}f$ we deduce that $V = J\,\mathrm{d}f$ on a neighborhood as desired.

Now suppose M is also simply connected. Then every closed one form is exact, and so $V \lrcorner \omega$ is closed if and only if $V \lrcorner \omega = \mathrm{d}f$ and $V = J\,\mathrm{d}f$ for a smooth function f defined on all of M. □

A smooth vector field V is called an **infinitesimal symmetry** of the Hamiltonian H if both ω and H are invariant under the flow e^{tV} of V. The second condition $(e^{tV})^*H = H$ can be recast as $V(H) = 0$, as can be seen by differentiating $H \circ e^{tV} = H$ with respect to t at $t = 0$. With this notion, we can prove the following analogue of Proposition 4.12.

Proposition 9.14 (Noether's theorem)**.** *Let (M, ω) be a symplectic manifold and H a fixed Hamiltonian. If f is a conserved quantity, then the Hamiltonian vector field $J\,\mathrm{d}f$ is an infinitesimal symmetry. Conversely, if M is also simply connected then each infinitesimal symmetry is the Hamiltonian vector field of a conserved quantity, and the quantity is unique up to the addition of a function that is constant on each component of M.*

Proof. First suppose f is a conserved quantity. Then from the identity (9.13) we know that $\{H, f\} = 0$. However, since the Poisson bracket is antisymmetric, we deduce that $0 = \{f, H\} = (J\,\mathrm{d}f)(H)$ as well. This demonstrates that H is conserved by $J\,\mathrm{d}f$ and from Theorem 9.6 we know that ω is also conserved by $J\,\mathrm{d}f$, and hence $J\,\mathrm{d}f$ is an infinitesimal symmetry.

Now suppose that M is simply connected and V is an infinitesimal symmetry. Then V is symplectic by definition, and by Proposition 9.13 we know V is globally Hamiltonian. Writing $V = J\,\mathrm{d}f$, since H is conserved by f then we have $0 = (J\,\mathrm{d}f)(H) = \{f, H\} = -\{H, f\}$, and therefore f is a conserved quantity. If g is another function with $J\,\mathrm{d}g = V = J\,\mathrm{d}f$, then by definition of J we have $\mathrm{d}(f - g) = (J\,\mathrm{d}f - J\,\mathrm{d}g) \lrcorner \omega = 0$ and hence $f - g$ is constant on the components of M. □

9.7. Exercises

9.1. Show that the following criteria for a nondegenerate two-form ω are equivalent.

(a) For each $x \in M$ the map $T_xM \to T_x^*M$ which takes $\xi \mapsto \omega(\xi, \cdot)$ is invertible.

(b) For each $x \in M$ and $\xi \in T_xM$ nonzero there exists $\eta \in T_xM$ such that $\omega(\xi, \eta) \neq 0$.

(c) The local matrix representation of ω in terms of some (hence every) basis is invertible.

9.2. Let $J^{ij}(x)$ denote the structure matrix of a non-degenerate Poisson bracket as in Corollary 7.9 and let $J_{ij}(x)$ denote the entries of the inverse matrix. Show that

$$\frac{\partial J_{ab}}{\partial x^c} + \frac{\partial J_{ca}}{\partial x^b} + \frac{\partial J_{bc}}{\partial x^a} = 0$$

for every triple of indices a, b, and c. Note that this implies that the 2-form (9.1) is closed. (Hint: Use the Jacobi identity (7.14) for J along with the derivative (A.15) of the determinant.)

9.3. (a) Show that rotation on the two-dimensional sphere S^2 is a Hamiltonian flow.

(b) Show that translations $g_t(q, p) = (q + t, p)$ on the torus $\mathbb{R}^2/\mathbb{Z}^2$ is a locally Hamiltonian flow, but is not globally Hamiltonian.

9.4. Let (M, ω) be a $2n$-dimensional compact symplectic manifold.

(a) Show that the n-fold wedge product ω^n is not exact.

(b) Show that the de-Rham cohomology groups $H^{2k}_{\mathrm{dR}}(M)$ are nontrivial for $k = 1, \ldots, n$.

(c) Conclude that the two-dimensional sphere S^2 is the only sphere that admits a symplectic structure.

9.5 (Symplectic and complex structure)**.** Identify Euclidean phase space $\mathbb{R}^{2n} = \mathbb{R}^n_q \times \mathbb{R}^n_p$ with the complex space $\mathbb{C}^n$ via $z_j := q_j + ip_j$.

(a) Show that matrix multiplication by matrix J (9.6) on $\mathbb{R}^{2n}$ corresponds to multiplication by $-i$ on $\mathbb{C}^n$. This is why the matrix (9.6) is called J, and in fact some authors (e.g. [Arn89]) choose the opposite sign for the canonical symplectic form (9.2) and use the notation I in place of J.

(b) Show that the Hermitian inner product $(z, w) \mapsto \sum z_j \overline{w}_j$ on $\mathbb{C}^n$ corresponds to $(\xi, \eta) \mapsto \xi \cdot \eta + i\, \xi \cdot J\eta$ on $\mathbb{R}^{2n}$. In other words, the scalar product and symplectic product are the real and imaginary parts of the Hermitian inner product, respectively.

9.6. (Hamiltonian PDE [Gar71]) The Hamiltonian mechanics we have developed thus far originates from the time derivative of trajectories in phase space and hence provides a class of ODEs on a finite dimensional manifold; however, this can be extended to PDE when we consider the time derivative of trajectories in an infinite dimensional function space. Given a smooth functional F of, say, smooth real-valued periodic functions $C^\infty(\mathbb{R}/\mathbb{Z})$ we denote the Fréchet derivative kernel by $\delta F/\delta q(x)$, so that

$$\mathrm{d}F\big|_q(f) = \frac{\mathrm{d}}{\mathrm{d}s}\bigg|_{s=0} F(q+sf) = \int \frac{\delta F}{\delta q}(x) f(x)\,\mathrm{d}x.$$

The Fréchet space $C^\infty(\mathbb{R}/\mathbb{Z};\mathbb{R})$ will now take the role of the manifold M. Specifically, for two smooth functionals $F(q)$ and $G(q)$ on $C^\infty(\mathbb{R}/\mathbb{Z})$ we define the Poisson bracket

$$\{F,G\} = \int \left(\frac{\delta F}{\delta q}\right)'(x) \frac{\delta G}{\delta q}(x)\,\mathrm{d}x.$$

In other words, we have replaced the dot product on the Euclidean phase space $\mathbb{R}^{2n}$ and the matrix J (9.6) with the L^2 real inner product and the skew-symmetric operator $J = \frac{\partial}{\partial x}$. Given a smooth functional $H(q)$ on $C^\infty(\mathbb{R}/\mathbb{Z})$, we define the associated Hamiltonian PDE

$$\frac{\partial q}{\partial t} = \frac{\partial}{\partial x}\left(\frac{\partial H}{\partial q}\right)$$

in the spirit of (9.4) and (9.13).

It turns out that many of the results of finite dimensional Hamiltonian mechanics have analogs in this infinite dimensional setting. For example, the global minimum of a classical Hamiltonian is a (Liapunov) stable equilibrium, and the global minimum of a Hamiltonian functional is orbitally stable (i.e. concentration compactness).

(a) Check that this Poisson bracket is bilinear, antisymmetric, and satisfies the Jacobi identity.

(b) Given a Hamiltonian functional $H(q)$, show that a smooth functional $F(q)$ is constant for solutions q to the PDE associated to H if and only if $\{H,F\} = 0$ as a functional on $C^\infty(\mathbb{R}/\mathbb{Z})$.

(c) Show that for any Hamiltonian functional $H(q)$ both the Hamiltonian H and the **mass functional**

$$M(q) := \int_0^1 q(x)\,\mathrm{d}x$$

are automatically conserved for solutions q to the PDE associated to H.

(d) Show that the **momentum functional**

$$P(q) := \tfrac{1}{2}\int_0^1 q(x)^2\,\mathrm{d}x$$

does indeed generate translations, in the sense that the solution to the associated PDE with initial data $q(0,x) = f(x)$ is $q(t,x) = f(x+t)$.

(e) The Korteweg–de Vries (KdV) equation is the PDE associated to the Hamiltonian

$$H_{\mathrm{KdV}}(q) := \int_0^1 \left(\tfrac{1}{2}q'(x)^2 - q(x)^3\right) \mathrm{d}x,$$

and arises as the long-wavelength and shallow-water limit for unidirectional water waves of height q from the undisturbed water level $q = 0$. Show that the mass $M(q)$, momentum $P(q)$, and energy $H_{\mathrm{KdV}}(q)$ are all constant for solutions q to KdV. In fact, these are the first three of an infinite hierarchy of conserved quantities for KdV.

CHAPTER 10

CONTACT GEOMETRY

Just as symplectic geometry extends the structure of conservative Hamiltonian dynamics on phase space, contact geometry is the natural generalization of nonconservative dynamics on the product of phase space with the time axis. The material for this chapter is based on [BCT17] and [Lee13, Ch. 22].

10.1. Contact structure

A **contact manifold** is a smooth $(2n+1)$-dimensional manifold M paired with a contact form η. A **contact form** η is a one-form required to satisfy the following nondegeneracy condition: for each $x \in M$ the restriction of $\mathrm{d}\eta_x$ to the subspace $\ker(\eta_x) \subset T_x M$ is nondegenerate (i.e. $\mathrm{d}\eta_x$ is a symplectic tensor for all $x \in M$). The rank-$2n$ distribution $N \subset TM$ satisfying $N_x = \ker(\eta_x)$ for each $x \in M$ is called a **contact structure** on M; it plays a fundamental role and is sometimes taken in the literature to be the defining geometric concept instead of η.

Similar to how the symplectic form nondegeneracy condition is equivalent to the nonvanishing of the n-fold wedge product $(\omega)^n$, this nondegeneracy condition turns out to be equivalent to

$$\eta \wedge (\mathrm{d}\eta)^n \neq 0; \tag{10.1}$$

the proof of this equivalence is Exercise 10.1. Consequently, $\eta \wedge (\mathrm{d}\eta)^n$ defines a volume form on M, and so in particular M must be orientable. Although the condition (10.1) is sometimes easily verifiable in practice, we will conceptually be relying on the first condition.

Example 10.1. On the Euclidean contact space $\mathbb{R}_S \times T^*\mathbb{R}^n = \mathbb{R}_S \times \mathbb{R}^n_q \times \mathbb{R}^n_p$ we have the **canonical contact form**

$$\eta = \mathrm{d}S - p\,\mathrm{d}q = \mathrm{d}S - \sum_{i=1}^{n} p^i\,\mathrm{d}q^i. \tag{10.2}$$

Note that this is the combination of $\mathrm{d}S$ and the tautological one-form (9.3) on $T^*\mathbb{R}^n$. A straightforward computation shows that $\eta \wedge (\mathrm{d}\eta)^n = \mathrm{d}S \wedge \mathrm{d}q \wedge \mathrm{d}p$ is the Euclidean volume form on $\mathbb{R}_t \times T^*\mathbb{R}^n$, but we can also check that $\mathrm{d}\eta$ is a

symplectic tensor. Note that $\mathrm{d}\eta = -\mathrm{d}p \wedge \mathrm{d}q$, and so the rank-$2n$ distribution $N \subset T\mathbb{R}^{2n+1}$ annihilated by η is spanned by the vector fields

$$X_i = \frac{\partial}{\partial q^i} + p^i \frac{\partial}{\partial S}, \qquad Y_i = \frac{\partial}{\partial p^i}$$

for $i = 1, \dots, n$. Moreover, we have

$$\mathrm{d}\eta(X_i, X_j) = 0, \qquad \mathrm{d}\eta(Y_i, Y_j) = 0, \qquad \mathrm{d}\eta(X_i, Y_j) = \delta_{ij}$$

for $i, j = 1, \dots, n$, and it follows that $\mathrm{d}\eta|_N$ is nondegenerate as in Example 9.2.

This example is again fundamental in the following sense.

Theorem 10.2 (Contact Darboux theorem)**.** *If (M, η) is a $(2n+1)$-dimensional contact manifold, then for each $x \in M$ there exist local coordinates (q, p, S) centered at x with respect to which η has the representation* (10.2)*.*

See [Lee13, Th. 22.31] for a proof.

The contact structure automatically induces an associated vector field called the Reeb field, which heuristically points orthogonally to the distribution N and plays the role of S-axis.

Proposition 10.3 (The Reeb field)**.** *If (M, η) is a contact manifold, then there exists a unique smooth vector field ξ on M called the* Reeb field *satisfying*

$$\xi \lrcorner \mathrm{d}\eta = 0, \qquad \eta(\xi) = 1. \tag{10.3}$$

Proof. The map Φ which takes $X \mapsto X \lrcorner \mathrm{d}\eta$ defines a smooth bundle homomorphism $\Phi : TM \to T^*M$, and for each $x \in M$ it reduces to a linear map $\Phi_x : T_xM \to T_x^*M$. As $\mathrm{d}\eta_x$ restricted to the subspace N_x is nondegenerate by definition, then $\Phi_x|_{N_x}$ is injective and hence Φ_x has rank at least $2n$. On the other hand, we know that Φ_x cannot have rank $2n+1$ because then $\mathrm{d}\eta_x$ would be nondegenerate and contradict that T_xM is odd-dimensional. Therefore, we conclude that $\ker \Phi_x$ is one-dimensional. Moreover, since $\ker(\Phi_x)$ is not contained in $N_x = \ker(\eta_x)$ by definition, we know there exists a unique $\xi \in \ker(\Phi_x)$ with $\eta_x(\xi_x) = 1$; these correspond to the two conditions (10.3) respectively.

The smoothness of ξ follows from the smoothness of η. Note that $\ker \Phi \subset TM$ is a smooth rank-one subbundle, and so around any $x \in M$ we can pick a smooth nonvanishing section X of $\ker \Phi$ near x. As $\eta(X) \neq 0$, then we can write $\xi = \eta(X)^{-1} X$ as a composition of smooth maps near x. □

Example 10.4. For the Euclidean contact space of Example 10.1, we see that Reeb field is

$$\xi = \frac{\partial}{\partial S}$$

as the two conditions (10.3) are easily verified.

10.2. Hamiltonian vector fields

Given a smooth function H on a contact manifold (M, η), the associated **contact Hamiltonian vector field** X_H is uniquely determined by the two conditions

$$\eta(X_H) = H, \qquad (X_H \lrcorner \mathrm{d}\eta)|_N = -\mathrm{d}H|_N. \tag{10.4}$$

As $\mathrm{d}\eta|_N$ is nondegenerate by definition, there is a unique vector field Y on N satisfying the second condition of (10.4). The vector field $X_H := Y + H\xi$ is then the unique solution of the conditions (10.4).

In comparison to symplectic Hamiltonian vector fields, the first condition of (10.4) looks like the primitive of $\omega(X_H) = \mathrm{d}H$ (which we wrote as $X_H = J\,\mathrm{d}H$) and the second condition is like $X_H \lrcorner \omega = \mathrm{d}H$; in the symplectic case these conditions were redundant (cf. (9.5)), but now we need both in order to determine X_H on and off of the kernel N_x of η_x.

Example 10.5. Let us see what the contact Hamiltonian vector field X_H looks like for the Euclidean contact space of Example 10.1 (and hence also the expression of X_H in the local coordinates guaranteed by Theorem 10.2). Given a smooth function $H(s, q, p)$ it is easily verified that

$$X_H = \sum_{i=1}^{n} \left(p^i \frac{\partial H}{\partial p^i} - H \right) \frac{\partial}{\partial S} + \frac{\partial H}{\partial p^i} \frac{\partial}{\partial q^i} - \left(\frac{\partial H}{\partial q^i} + p^i \frac{\partial H}{\partial S} \right) \frac{\partial}{\partial p^i} \tag{10.5}$$

satisfies the two conditions (10.4), from which we obtain the differential equation system

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \sum_{i=1}^{n} p^i \frac{\partial H}{\partial p^i} - H, \qquad \frac{\mathrm{d}q^i}{\mathrm{d}t} = \frac{\partial H}{\partial p^i}, \qquad \frac{\mathrm{d}p^i}{\mathrm{d}t} = -\frac{\partial H}{\partial q^i} - p^i \frac{\partial H}{\partial S}. \tag{10.6}$$

When H is independent of s, the second two sets of equations reduce to Hamilton's equations of motion (7.2). We also recognize the quantity S as the action $S(q, t)$; indeed, if we use the formula (6.1) for the momentum and use the Hamilton–Jacobi equation (6.4) we see that the time derivative of the action is

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \sum_{i=1}^{n} \frac{\partial S}{\partial q^i} \frac{\mathrm{d}q^i}{\mathrm{d}t} + \frac{\partial S}{\partial t} = \sum_{i=1}^{n} p^i \frac{\mathrm{d}q^i}{\mathrm{d}t} - H.$$

To conclude the section, let us consider a one-dimensional physical example for to illustrate how contact geometry encapsulates time-independent nonconservative dynamics.

Example 10.6. Take $n = 1$ in the Euclidean contact space of Example 10.1, and consider the Hamiltonian

$$H(q, p, S) = \frac{p^2}{2m} + V(q) + \gamma S \tag{10.7}$$

where γ is a real constant. The contact Hamilton's equations (10.6) read

$$\dot{q} = \frac{p}{m}, \qquad \dot{p} = -V'(q) - \gamma p, \qquad \dot{S} = \frac{p^2}{2m} - V(q) - \gamma S.$$

This represents a Newtonian system with a friction force that depends linearly on the velocity, like the damped harmonic oscillator of Example 2.9. Note that as opposed to Example 9.12, in this approach the momentum coordinate still coincides with the physical momentum defined via the velocity.

10.3. Dynamics

Using the expression (10.5) of a contact Hamiltonian vector field X_H in terms of the local coordinates (q, p, S) of Theorem 10.2, we see that a smooth function $F(q, p, S)$ on a contact manifold (M, η) evolves according to

$$\begin{aligned} \frac{\mathrm{d}F}{\mathrm{d}t} &= X_H(F) \\ &= -H\frac{\partial F}{\partial S} + \sum_{i=1}^{n} p^i \left[\frac{\partial H}{\partial p^i}\frac{\partial F}{\partial S} - \frac{\partial H}{\partial S}\frac{\partial F}{\partial p^i}\right] + \sum_{i=1}^{n}\left[\frac{\partial H}{\partial p^i}\frac{\partial F}{\partial q^i} - \frac{\partial H}{\partial q^i}\frac{\partial F}{\partial p^i}\right] \\ &= -H\frac{\partial F}{\partial S} + \sum_{i=1}^{n} p^i \{H, F\}_{p^i, S} + \{H, F\}_{p,q}. \end{aligned} \tag{10.8}$$

The last term above we recognize from (7.9) and the first two terms are corrections introduced by the contact structure. The notation $\{H, F\}_{p^i,S}$ should be interpreted as a convenient shorthand defined via the above formula with no deeper meaning.

Taking $F = H(q, p, S)$ to be the Hamiltonian for the vector field X_H in the formula (10.8) above, we see that the Hamiltonian evolves according to

$$\frac{\mathrm{d}H}{\mathrm{d}t} = -H\frac{\partial H}{\partial S}. \tag{10.9}$$

From this we see that H is a conserved quantity if and only if H is independent of S or $H = 0$. In particular, for a conservative Hamiltonian $H \equiv H(q, p)$ we recover the conservation of the Hamiltonian. However, in general the rate of decrease of the Hamiltonian is proportional to the system's energy H and its dissipation $\partial H/\partial S$.

Specifically, let us consider a Hamiltonian of the form

$$H(q, p, S) = H_0(q, p) + f(S) \tag{10.10}$$

where $H_0(q, p)$ is the mechanical energy of the system (e.g. $H_0(q, p) = p^2/2m + V(q)$), then according to the formula (10.8) the mechanical energy obeys

$$\frac{\mathrm{d}H_0}{\mathrm{d}t} = -\sum_{i=1}^{n} p^i \frac{\partial H_0}{\partial p^i} f'(S). \tag{10.11}$$

We interpret this as saying that $f(S)$ is the potential for the system's dissipative force. Moreover, the evolution (10.9) of the Hamiltonian can be integrated to obtain

$$H(t) = H(0) \exp\left[- \int_0^t f'(S) \right].$$

Plugging in the Hamiltonian (10.10), we obtain an implicit equation which in principle determines the action $S = S(q, p, t)$; thus the equations of motion (10.6) reduce to the $2n$ equations for the positions q^i and momenta p^i.

Example 10.7. If we take $d = 1$ and the dissipative potential $f(S) = \gamma S$ to be linear as in Example 10.6 then equation (10.11) becomes

$$\dot{H}_0 = -m\gamma \dot{q}^2$$

which agrees with what we found for the damped harmonic oscillator of Example 2.9. The energy of this system decays exponentially to zero, according to

$$H(t) = H(0) e^{-\gamma t}.$$

Solving for the action S we obtain

$$S(q, p, t) = \frac{1}{\gamma} \left[H(0) e^{-\gamma t} - \frac{p^2}{2m} - V(q) \right].$$

10.4. Contact transformations

A **contact transformation** is a smooth transformation which leaves the contact structure invariant. As opposed to canonical transformations, we allow the contact form $f\eta$ in the new coordinates to differ by a smooth nonvanishing factor $f \in C^\infty(M)$ since we are interested in the contact structure N. In terms of the canonical coordinates (q, p, S) guaranteed by Theorem 10.2, the new coordinates $(\tilde{q}, \tilde{p}, \tilde{S})$ must satisfy

$$\tilde{\eta} = \mathrm{d}\tilde{S} - \tilde{p}\, \mathrm{d}\tilde{q} = f(\mathrm{d}S - p\, \mathrm{d}q) = f\eta. \tag{10.12}$$

Writing $(\tilde{S}, \tilde{q}, \tilde{p})$ as functions of (q, p, S), this is equivalent to the conditions

$$f = \frac{\partial \tilde{S}}{\partial S} - \sum_{j=1}^n \tilde{p}^j \frac{\partial \tilde{q}^j}{\partial S}, \qquad -f p^i = \frac{\partial \tilde{S}}{\partial q^i} - \sum_{j=1}^n \tilde{p}^j \frac{\partial \tilde{q}^j}{\partial q^i}, \qquad 0 = \frac{\partial \tilde{S}}{\partial p^i} - \sum_{j=1}^n \tilde{p}^j \frac{\partial \tilde{q}^j}{\partial p^i}$$

for $i = 1, \dots, d$. Note that canonical transformations are independent of $S, \tilde{S}$ and are defined by the condition (10.12) with $f \equiv 1$.

As we allow for a conformal factor f in the definition (10.12), the volume form is also rescaled. Indeed, if $\tilde{\eta} = f\eta$ then $\mathrm{d}\tilde{\eta} = \mathrm{d}f \wedge \eta + f\, \mathrm{d}\eta$, and so

$$\tilde{\eta} \wedge (\mathrm{d}\tilde{\eta})^n = f^{d+1} \eta \wedge (\mathrm{d}\eta)^n$$

is the new volume form. In the case of canonical transformations we have $f \equiv 1$, and hence we recover volume preservation.

As with canonical transformations in section 7.6, we may consider a contact transformation as being generated by a generating function. For an example, assume that the coordinates $(q, \tilde{q}, S)$ are independent. Then the differential of the generating function $\tilde{S} = \tilde{S}(q, \tilde{q}, S)$ may be written

$$\mathrm{d}\tilde{S} = \frac{\partial \tilde{S}}{\partial S}\,\mathrm{d}S + \sum_{i=1}^{n} \frac{\partial \tilde{S}}{\partial q^i}\,\mathrm{d}q^i + \sum_{i=1}^{n} \frac{\partial \tilde{S}}{\partial \tilde{q}^i}\,\mathrm{d}\tilde{q}^i.$$

Plugging this into (10.12), we see that the remaining coordinates are determined in terms of $\tilde{S}$ by

$$f = \frac{\partial \tilde{S}}{\partial S}, \qquad f p^i = -\frac{\partial \tilde{S}}{\partial q^i}, \qquad \tilde{p}^i = \frac{\partial \tilde{S}}{\partial \tilde{q}^i}.$$

Taking $f \equiv 1$, we see that $\tilde{S}$ is related to the canonical transformation generating function $F(q, \tilde{q})$ via

$$\tilde{S} = S - F(q, \tilde{q}).$$

In particular, we conclude that all physicist's time-independent canonical transformations (cf. the remark of section 7.6) are a special case of contact transformations.

Recall that for symplectic structures the Hamiltonian dynamics generate instantaneous canonical transformations by Proposition 9.13. In analogy with symplectic vector fields, we will call a smooth vector field V on M if a **contact vector field** if its flow e^{tV} preserves the contact structure N, in that

$$\mathrm{d}\big(e^{tV}\big)_x (N_x) = N_{e^{tV}x} \tag{10.13}$$

for all $t \in \mathbb{R}$ and $x \in M$ in the domain of definition of the flow e^{tV}.

Proposition 10.8. *Let (M, η) be a contact manifold. A smooth vector field V on M is a contact vector field if and only if it is a contact Hamiltonian vector field.*

Proof. From the condition (10.13) and the definition of the Lie derivative, we see that V is a contact vector field if and only if $\mathcal{L}_V \eta = 0$ on N.

First assume that V is a contact Hamiltonian vector field, and write $V = X_H$ for a Hamiltonian H. Then from Cartan's magic formula and the first condition (10.4) defining X_H we have

$$\mathcal{L}_{X_H}\eta = \mathrm{d}\left[\eta(X_H)\right] + X_H \lrcorner \mathrm{d}\eta = \mathrm{d}H + X_H \lrcorner \mathrm{d}\eta.$$

From the second condition of (10.4) we know that $X_H \lrcorner \mathrm{d}\eta$ is equal to $-\mathrm{d}H$ on N. By the definition (10.3) of the Reeb field it then follows that

$$\mathcal{L}_{X_H}\eta = -\xi(H)\eta = -\frac{\partial H}{\partial S}\eta, \tag{10.14}$$

where the last equality is merely the expression in terms of the local canonical coordinates. Comparing this to the definition (10.12) of a contact transformation, we see that the flow is a contact transformation with $f = -\xi(H) = -\partial H/\partial S$. In particular, if we restrict to the contact structure N, we have $\eta = 0$ and hence $\mathcal{L}_{X_H}\eta = 0$ as desired.

Conversely, assume that V is contact vector field. Then Cartan's magic formula reads

$$0 = (\mathcal{L}_V\eta)|_N = \mathrm{d}^{\eta(X_H)}|_N + (V \lrcorner \mathrm{d}\eta)|_N.$$

Consider the smooth function $H = \eta(V)$, defined so that the first condition of the definition (10.4) holds. Then we obtain the second condition of (10.4) from the above equality, and so we conclude that $V = X_H$ is the contact Hamiltonian vector field for H. □

Heuristically, we do not expect the volume form to be preserved by a general contact Hamiltonian flow since contact dynamics includes dissipative systems. Using (10.14) we see that the volume form evolves according to

$$\begin{aligned}\mathcal{L}_{X_H}[\eta \wedge (\mathrm{d}\eta)^n] &= (\mathcal{L}_{X_H}\eta) \wedge (\mathrm{d}\eta)^n + \sum_{i=0}^{n-1} \eta \wedge (\mathrm{d}\eta)^i \wedge [\mathrm{d}(\mathcal{L}_{X_H}\eta)] \wedge (\mathrm{d}\eta)^{n-1-i} \\ &= -(n+1)\frac{\partial H}{\partial S}\, \eta \wedge (\mathrm{d}\eta)^n.\end{aligned}$$

This illustrates the connection between the Hamiltonian's S-dependence to the system's dissipation, and consequently systems for which $\frac{\partial H}{\partial S}$ is nonvanishing are called **dissipative**.

Instead, we have a variant of Liouville's theorem due to [BT15], in which a rescaled volume form is preserved away from the zero set $H^{-1}(0)$.

Proposition 10.9 (Canonical measure for dissipative contact systems)**.** *Let (M, η) be a $(2n+1)$-dimensional contact manifold and H a smooth function on M. Then the volume form*

$$|H|^{-(n+1)}\, \eta \wedge (\mathrm{d}\eta)^n$$

is an invariant measure for the contact Hamiltonian flow for H along orbits outside of $H^{-1}(0)$. Moreover, up to scalar multiplication it is the unique such measure whose density with respect to the standard volume form depends only on H.

Proof. For a smooth function ρ on M, a computation using (10.14) shows that

$$\begin{aligned}\mathcal{L}_{X_H}[\rho\, \eta \wedge (\mathrm{d}\eta)^n] &= (\mathcal{L}_{X_H}\rho)\, \eta \wedge (\mathrm{d}\eta)^n - (n+1)\frac{\partial H}{\partial S}\rho\, \eta \wedge (\mathrm{d}\eta)^n \\ &= \left[X_H(\rho) - (n+1)\frac{\partial H}{\partial S}\rho\right]\, \eta \wedge (\mathrm{d}\eta)^n.\end{aligned}$$

If we assume $\rho = \rho(H)$ then

$$X_H(\rho) = -H\rho'(H)\frac{\partial H}{\partial S},$$

and so the vanishing of $\mathcal{L}_{X_H}[\rho\,\eta \wedge (\mathrm{d}\eta)^n]$ occurs exactly when ρ solves

$$\rho'(H) = -(n+1)H^{-1}\rho.$$

This equation has the solution $\rho(H) = |H|^{-(n+1)}$ and it is unique up to scalar multiplication. □

10.5. Time-dependent systems

Thus far we have allowed H to be a function on the contact manifold M, and hence have only considered time-independent dissipative systems. In this section, we present the extension introduced in [BCT17] of contact Hamiltonian systems to include time-dependence.

For (M, η) a $(2n+1)$-dimensional contact manifold, we define the **extended manifold** $M \times \mathbb{R}$. In analogy with the Poincaré–Cartan one-form (9.16), given a possibly time-dependent Hamiltonian H we extend the contact form to

$$\theta = \mathrm{d}S - p\,\mathrm{d}q + H\,\mathrm{d}t = \mathrm{d}S - \sum_{i=1}^{n} p^i\,\mathrm{d}q^i + H\,\mathrm{d}t \tag{10.15}$$

in terms of the canonical coordinates (q, p, S) on M guaranteed by Theorem 10.2.

On $M \times \mathbb{R}$ we define the **extended contact Hamiltonian vector field**

$$Y_H = X_H + \frac{\partial}{\partial t}.$$

In place of the conditions (10.4), it can be checked that this vector field is uniquely determined by

$$\theta(Y_H) = 0, \qquad Y_H \lrcorner \mathrm{d}\theta = -\frac{\partial H}{\partial S}\theta. \tag{10.16}$$

Here, the first condition is analogous to how (9.18) replaced (9.5) for time-dependent symplectic systems, and the second condition is the analog of (10.14) (which serves as a rephrasing for the second condition of (10.4) that does not involve N).

The flow of Y_H is given by

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \sum_{i=1}^{n} p^i\frac{\partial H}{\partial p^i} - H, \qquad \frac{\mathrm{d}q^i}{\mathrm{d}t} = \frac{\partial H}{\partial p^i}, \qquad \frac{\mathrm{d}p^i}{\mathrm{d}t} = -\frac{\partial H}{\partial q^i} - p^i\frac{\partial H}{\partial S}, \qquad \dot{t} = 1,$$

which are the old equations of motion (10.6) joined with the trivial equation $\dot{t} = 1$. It follows that any smooth time-dependent function F on $M \times \mathbb{R}$ evolves according to

$$\frac{\mathrm{d}F}{\mathrm{d}t} = -H\frac{\partial F}{\partial S} + \sum_{i=1}^{n} p^i\{H, F\}_{p^i,S} + \{H, F\}_{p,q} + \frac{\partial F}{\partial t}, \tag{10.17}$$

using the notation of eq. (10.8). In particular, we see that under its own flow the Hamiltonian now changes according to both its dissipation $\partial H/\partial S$ and its time-dependence.

Lastly, let us extend the notion of contact transformations to our extended manifold $M\times\mathbb{R}$. In terms of canonical coordinates, a **time-dependent contact transformation** $(q,p,S,t)\mapsto(\tilde{q},\tilde{p},\tilde{S},\tilde{t})$ must satisfy

$$\tilde{\theta}=\mathrm{d}\tilde{S}-\tilde{p}\,\mathrm{d}\tilde{q}+K\,\mathrm{d}\tilde{t}=f(\mathrm{d}S-p\,\mathrm{d}q+H\,\mathrm{d}t)=f\theta \tag{10.18}$$

for a smooth nonvanishing factor $f\in C^\infty(M\times\mathbb{R})$ and a new Hamiltonian $K\in C^\infty(M\times\mathbb{R})$. Expanding $\mathrm{d}\tilde{q}$ and $\mathrm{d}\tilde{S}$, we see that the new Hamiltonian must satisfy

$$fH=\frac{\partial\tilde{S}}{\partial t}-\sum_{i=1}^{n}\tilde{p}^i\frac{\partial\tilde{q}^i}{\partial t}+K.$$

As before, we may consider a contact transformation as being generated by a generating function. For example, let us assume that the coordinates $(q,\tilde{q},S,t)$ are independent. After substituting the differential of the generating function $\tilde{S}=\tilde{S}(q,\tilde{q},S,t)$ into (10.18), we see that the remaining coordinates are determined in terms of $\tilde{S}$ by

$$f=\frac{\partial\tilde{S}}{\partial S},\qquad fp^i=-\frac{\partial\tilde{S}}{\partial q^i},\qquad \tilde{p}^i=\frac{\partial\tilde{S}}{\partial\tilde{q}^i},\qquad fH=\frac{\partial\tilde{S}}{\partial t}+K. \tag{10.19}$$

The first three conditions are unchanged and the last condition defines the new Hamiltonian $K=K(q,\tilde{q},S,t)$. Taking $f\equiv 1$, we see that $\tilde{S}$ is related to the canonical transformation generating function $F(q,\tilde{q},t)$ via

$$\tilde{S}=S-F(q,\tilde{q},t).$$

However, now there is an additional constraint on $\tilde{S}$ imposed by the invariance of the second condition of (10.16). After the transformation we must have

$$Y_H\lrcorner\mathrm{d}\theta=-\frac{\partial K}{\partial\tilde{S}}\tilde{\theta}.$$

Using $\tilde{\theta}=f\theta$, $\tilde{Y}_H=Y_H$, and the extended contact Hamiltonian vector field conditions (10.16), this yields

$$f\frac{\partial K}{\partial\tilde{S}}=f\frac{\partial H}{\partial S}+\mathrm{d}f(Y_H).$$

In the special case $f\equiv 1$ we note that if H is independent of S then $K=0$ is a solution, in which case the last condition of (10.19) becomes the familiar Hamilton–Jacobi equation (6.4). However, in general f may be S-dependent and so the notion of contact transformations is strictly more general than even the physicist's notion of canonical transformations (cf. the remark of section 7.6).

Example 10.10. In Example 9.12 we introduced a non-canonical coordinate transformation $(q,p) \mapsto (q, e^{\gamma t})$ to describe a dissipative system using time-dependent Hamiltonian dynamics. However, it is easily checked that the transformation

$$\tilde{q} = q, \qquad \tilde{p} = e^{\gamma t} p, \qquad \tilde{S} = e^{\gamma t} S, \qquad \tilde{t} = t$$

satisfies eq. (10.15) and is hence a time-dependent contact transformation. Here, the conformal factor is $f = e^{\gamma t}$, and the Hamiltonians are expressed in their respective coordinates: H is given by eq. (10.7) and K is given by eq. (9.20).

10.6. Exercises

10.1. Show that a smooth one-form η on a $(2n+1)$-dimensional manifold M satisfies the nondegeneracy condition of a contact form if and only if it satisfies the nonvanishing top form condition (10.1).

10.2 (Contact structure on S^{2n+1})**.** On the Euclidean space $\mathbb{R}^{2n+2}$ consider the coordinates $(x^1, \dots, x^{n+1}, y^1, \dots, y^{n+1})$ and define the one-form

$$\theta := \sum_{i=1}^{n+1} \left(x^i \, \mathrm{d}y^i - y^i \, \mathrm{d}x^i \right).$$

The **standard contact form** on the sphere S^{2n+1} is $\eta := \iota^* \theta$, where $\iota := : S^{2n+1} \hookrightarrow \mathbb{R}^{2n+2}$ is the inclusion map.

(a) Show that the vector fields

$$V = \sum_{i=1}^{n+1} \left(x^i \frac{\partial}{\partial x^i} + y^i \frac{\partial}{\partial y^i} \right), \qquad W = \sum_{i=1}^{n+1} \left(x^i \frac{\partial}{\partial y^i} - y^i \frac{\partial}{\partial x^i} \right)$$

satisfy $V \lrcorner \mathrm{d}\theta = 2\theta$ and $W \lrcorner \mathrm{d}\theta = -\,\mathrm{d}\big(x^2 + y^2\big)$.

(b) Let $S \subset T(\mathbb{R}^{2n+1} \setminus \{0\})$ denote the subbundle spanned by V and W, and let

$$S^\perp = \bigcup_{p \in S^{2n+1}} \big\{ X \in T_p \mathbb{R}^{2n+2} : \mathrm{d}\theta_p(V_p, X_p) = \mathrm{d}\theta_p(W_p, X_p) = 0 \big\}$$

denote its symplectic complement. Show that θ is indeed a contact form with respect to the contact structure $S^\perp$.

(c) Show that the corresponding Reeb field is given by W restricted S^{2n+1}.

10.3 (Solving the damped parametric oscillator via expanding coordinates)**.** Consider the one-dimensional damped parametric oscillator

$$H = \frac{p^2}{2m} + \frac{m}{2} \omega^2(t) q^2 + \gamma S$$

with time-dependent frequency $\omega(t)$ and damping parameter γ. Show that the new **expanding coordinates**

$$\tilde{q} = e^{\gamma t/2} q, \qquad \tilde{p} = e^{\gamma t/2}(p + \tfrac{1}{2} m\gamma q), \qquad \tilde{S} = e^{\gamma t}(S + \tfrac{1}{4} m\gamma q^2), \qquad \tilde{t} = t$$

define a contact transformation, with respect to which the Hamiltonian takes the form

$$K = \frac{\tilde{p}^2}{2m} + \frac{m}{2}\left(\omega^2(t) - \tfrac{1}{4}\gamma^2\right)\tilde{q}^2.$$

This new Hamiltonian K now corresponds to an undamped parametric oscillator with the new frequency $\sqrt{\omega^2(t) - \frac{1}{4}\gamma^2}$. The undamped oscillator has been extensively studied and solutions for the equations of motion can be obtained. In the harmonic oscillator case $\omega(t) \equiv \omega_0$ the Hamiltonian K is a conserved quantity, and the coordinates expand exponentially in time so that the trajectories form closed orbits at a slower frequency.

10.4 (Solving the damped parametric oscillator via conserved quantities)**.** Consider the one-dimensional damped parametric oscillator

$$H = \frac{p^2}{2m} + \frac{m}{2}\omega^2(t) q^2 + \gamma S$$

with time-dependent frequency $\omega(t)$ and damping parameter γ.

(a) We seek a solution F to eq. (10.17) with vanishing left-hand side. Substituting the quadratic ansatz

$$F(q, p, S, t) := \beta(t) p^2 - 2\xi(t) qp + \eta(t) q^2 + \zeta(t) S,$$

obtain a system of first-order equations for β, η, ξ, and ζ, where the $\dot{\zeta}$ has solution $\zeta(t) = \zeta_0 e^{\gamma t}$.

(b) Using the substitution $\beta(t) := \frac{1}{2m} e^{\gamma t} \alpha^2(t)$, show that the β equation is solved if and only if α satisfies the Ermakov equation

$$\ddot{\alpha} + [\omega^2(t) - \tfrac{1}{4}\gamma^2]\alpha = \alpha^{-3},$$

and the remaining equations become

$$\eta(t) = \tfrac{1}{2} m e^{\gamma t}\{[\dot{\alpha} - \tfrac{1}{2}\gamma\alpha]^2 + \alpha^{-2}\}, \qquad \xi(t) = \tfrac{1}{2} e^{\gamma t}[\dot{\alpha} - \tfrac{1}{2}\gamma\alpha] + \tfrac{1}{4}.$$

(c) Conclude that the quantity $F(q, p, S, t) = I(q, p, t) + \zeta_0 G(q, p, S, t)$ is conserved, with

$$I = \frac{m}{2} e^{\gamma t}\left\{\left[\frac{p}{m}\alpha - \left(\dot{\alpha} - \frac{\gamma}{2}\alpha\right) q\right]^2 + \left(\frac{q}{\alpha}\right)^2\right\}, \qquad G = e^{\gamma t}(S - \tfrac{1}{2} qp),$$

and $\alpha(t)$ solves the Ermakov equation. Moreover, since F is invariant for all initial conditions and ζ_0 is determined solely by initial conditions, then I and G must be separately conserved.

(d) Show that the new coordinates

$$\tilde{q} = \arctan\left[(\dot{\alpha} - \tfrac{1}{2}\gamma\alpha)\alpha - \alpha^2 \frac{p}{mq}\right], \quad \tilde{p} = I(q,p,t), \quad \tilde{S} = G(q,p,S,t),$$

(and $\tilde{t} = t$) define a contact transformation, with respect to which the new Hamiltonian is simply $K = I\alpha^{-2}$. Solve the new equations of motion for $\tilde{q}, \tilde{p}, \tilde{S}$ and obtain the solution

$$q(t) = \sqrt{\frac{2I}{m}} e^{\gamma t}\alpha(t)\cos\phi(t), \qquad S(t) = Ge^{-\gamma t} + \tfrac{1}{2}q(t)p(t),$$
$$p(t) = \sqrt{2mI}e^{\gamma t}\left[\left(\dot{\alpha} - \frac{\gamma}{2}\alpha\right)\cos\phi(t) - \frac{1}{\alpha}\sin\phi(t)\right], \qquad \phi(t) = \int_{t_0}^{t} \frac{\mathrm{d}\tau}{\alpha^2(\tau)}.$$

Here, $\alpha(t)$ solves the Ermakov equation and the conserved quantities I and G are determined by the initial conditions.

APPENDIX A

FUNDAMENTALS OF ODE THEORY

We collect some facts from introductory ODE theory in this chapter for easy reference. The material is based on [CL55].

A.1. Picard iteration

Throughout this chapter, we will study the **initial value problem** (IVP)

$$\dot{x} = f(t, x(t)), \qquad x(0) = x_0, \tag{A.1}$$

where $\dot{g} = \frac{\mathrm{d}g}{\mathrm{d}t}$ denotes a time derivative. The equation (A.1) describes the evolution of a point x, which we will take to lie in a Banach space $(X, |\cdot|)$. Although we will primarily be concerned with the case $X = \mathbb{R}^d$ in these notes, this level of generality is useful as it includes some systems with infinite degrees of freedom (e.g. Example 7.29 and section 8.6). However, this is not broad enough to really include PDE, except for some boring examples.

Our first step will be to recast the IVP (A.1) as an integral equation:

Lemma A.1. *If $f : \mathbb{R} \times X \to X$ is continuous, then the following are equivalent:*

(a) (Classical solution) $x : (-T, T) \to X$ is C^1 and solves the IVP (A.1)*.*

(b) (Strong solution) $x : (-T, T) \to X$ is C^0 and solves the integral equation

$$x(t) = x(0) + \int_0^t f(s, x(s))\,\mathrm{d}s. \tag{A.2}$$

Proof. Both directions easily follow from the fundamental theorem of calculus.

First assume that (a) holds. Then both sides of the IVP (A.1) are continuous, and so integration yields (A.2) by the fundamental theorem of calculus.

Now assume that (b) holds. Then $t \mapsto f(t, x(t))$ is continuous, and so by the fundamental theorem of calculus the integral equation (A.2) says that x is differentiable with derivative $f(t, x(t))$. □

In the case $X = \mathbb{R}^d$, we can give a more general measure-theoretic version of Lemma A.1 via the following statement of the fundamental theorem of calculus:

given $g : (-T, T) \to \mathbb{R}^d$ in L^1, the function $x : (-T, T) \to \mathbb{R}^d$ is absolutely continuous and solves $\dot{x}(t) = g(t)$ almost everywhere iff $x(t) = x(0) + \int_0^t g(s)\,\mathrm{d}s$. The theory of absolute continuity for Banach-valued functions exists, but is quite involved.

Lemma A.1 does not apply to many PDE, not even to the transport equation $\frac{\partial u}{\partial t} = \frac{\partial u}{\partial x}$, because spatial differentiation $u \mapsto \frac{\partial u}{\partial x}$ is not continuous in most Banach spaces. (There are some exceptions to this though, like the space of holomorphic functions on a strip $\{z \in \mathbb{C} : |\operatorname{Im} z| < c\}$ containing the real axis.) Moreover, the conclusion of Lemma A.1 does not hold, and (a) and (b) yield distinct notions of solutions. Another common notion is that of weak solutions: an L^∞ function $x : (-T, T) \to X$ that solves

$$\int_{-T}^{T} x(t)\psi(t)\,\mathrm{d}t = x(0)\int_{-T}^{T} \psi(t)\,\mathrm{d}t + \int_{-T}^{T} \psi(t)\int_0^t f(s, x(s))\,\mathrm{d}s\,\mathrm{d}t$$

for all $\psi \in C_0^\infty([-T, T])$. For ODEs, it turns out that this is also equivalent provided that f is continuous, but we will not need this fact.

In trying to argue that solutions to the IVP (A.1) exist, the formulation (b) is better than that of (a). This is because integrals are stable while derivatives are highly unstable. For example, consider the Fourier series $g(t) = \sum_{k\neq 0} c_k e^{2\pi i k t}$. If the coefficients c_k are absolutely summable, then this defines a periodic function $g(t)$. Roughly speaking, the rate of decay of c_k corresponds to the smoothness of $g(t)$, because the character $e^{2\pi i k t}$ is rapidly oscillating for large frequencies k. Integration suppresses high frequencies, because it replaces the coefficients of $g(t)$ by more rapidly decaying sequence $\frac{c_k}{2\pi i k}$. Conversely, differentiation amplifies high frequencies, because it replaces the coefficients of $g(t)$ by more slowly decaying sequence $2\pi i k c_k$.

In addition to differential equations, the theory of integral equations also exists. The integral equation (A.2) is special in that the integration is over $[0, t]$, and such equations are said to be of Volterra type (in analogy with triangular matrices). The more general case

$$x(t) = b(t) + \int_0^1 K(t, s)x(s)\,\mathrm{d}s$$

is called a Fredholm integral equation, of which the linear case is shown above.

The following theorem is a fundamental result on the existence of solutions:

Theorem A.2 (Picard–Lindelöf)**.** *If $f : \mathbb{R} \times X \to X$ is continuous and is Lipschitz in x:*

$$|f(t, x) - f(t, y)| \le C|x - y| \quad \text{for all } x, y \in X \tag{A.3}$$

for some constant $C > 0$, then for each $x_0 \in X$ there exists a unique continuous function $x : \mathbb{R} \to X$ so that the integral equation (A.2) *holds. Moreover, $x \in C([-T, T] \to X)$ depends continuously upon $x_0 \in X$ for all $T > 0$.*

Theorem A.2 says that the ODE (A.1) is (globally-in-time) **well-posed** (in the sense of Hadamard): solutions exist, solutions are unique, and solutions depend continuously upon the initial data. The statement of continuous dependence can take various forms; for example, it follows that given a convergent sequence of initial data, the corresponding sequence of solutions converges uniformly on compact time intervals. Note that continuous dependence upon initial data is not extremely restrictive; indeed, chaotic systems, where trajectories exhibit complex geometric structure and are sensitive to small changes in initial conditions, can still be well-posed.

We will only present one proof of Theorem A.2, but there are multiple arguments that apply. Having multiple methods is particularly useful in the study of PDEs, because different ODE proofs yield distinct PDE statements.

Proof. We will argue by Picard iteration. Recursively define the sequence

$$x_0(t) \equiv x_0, \qquad x_{n+1}(t) = x_0 + \int_0^t f(s, x_n(s))\,\mathrm{d}s$$

of successive approximate solutions. Ultimately we will show $\{x_n\}$ is a Cauchy sequence, and we will take its limit to be our solution.

We want to show that the difference between successive approximations is shrinking. Using the Lipschitz condition (A.3), we estimate

$$\begin{aligned} |x_{n+1}(t) - x_n(t)| &\le \int_0^t |f(s, x_n(s)) - f(s, x_{n-1}(s))|\,\mathrm{d}s \\ &\le C \int_0^t |x_n(s_n) - x_{n-1}(s_n)|\,\mathrm{d}s_n. \end{aligned}$$

We now have the difference between the previous two approximations on the RHS. Applying this estimate iteratively to the RHS, we obtain

$$\begin{aligned} &\le C^2 \int_0^t \int_0^{s_n} |x_{n-1}(s_{n-1}) - x_{n-2}(s_{n-1})|\,\mathrm{d}s_{n-1}\,\mathrm{d}s_n \\ &\vdots \\ &\le C^n \int_{0<s_1<s_2<\cdots<s_n<t} |x_1(s_1) - x_0(s_1)|\,\mathrm{d}s_1\,\mathrm{d}s_2 \ldots \mathrm{d}s_n. \end{aligned}$$

For the first two functions in our sequence, we can bound

$$|x_1(s_1) - x_0(s_1)| = \left| \int_0^{s_1} f(s_0, x_0)\,\mathrm{d}s_0 \right| \le s_1 \sup_{s\in(0,t)} |f(s, x_0)|.$$

Together, this yields

$$|x_{n+1}(t) - x_n(t)| \le \sup_{s\in(0,t)} |f(s, x_0)|\ \frac{C^n t^{n+1}}{(n+1)!}.$$

The RHS is summable in n, and so we conclude that $\{x_n(t)\}$ is a Cauchy sequence in $C([-T,T] \to X)$.

Define x to be the limit of x_n in $C([-T,T] \to X)$, which exists because X is complete. As x_n converges to x in this space, we have

$$\sup_{t\in[-T,T]} |x_n(t) - x(t)| \to 0 \quad \text{as } n \to \infty$$

for all $T > 0$. To see that $x(t)$ solves the IVP (A.1), we take $n \to \infty$ in the definition

$$x_{n+1}(t) = x_0 + \int_0^t f(s, x_n(s))\,\mathrm{d}s.$$

We have $f(s, x_n(s)) \to f(s, x(s))$ by continuity, so the integrals converge, and hence we obtain

$$x(t) = x_0 + \int_0^t f(s, x(s))\,\mathrm{d}s.$$

Therefore $x(t)$ is a solution to the integral equation (A.2), and consequently the IVP (A.1) by Lemma A.1.

Next, we claim that the solution is unique. Suppose $x(t)$ and $\tilde{x}(t)$ are both solutions to the IVP (A.1) that are in $C([-T,T] \to X)$. Arguing as before, we estimate

$$\begin{aligned}
|x(t) - \tilde{x}(t)| &\le \int_0^t |f(s, x(s)) - f(s, \tilde{x}(s))|\,\mathrm{d}s \\
&\le C \int_0^t |x(s_n) - \tilde{x}(s_n)|\,\mathrm{d}s_n \\
&\le C^2 \int_0^t \int_0^{s_n} |x(s_{n-1}) - \tilde{x}(s_{n-1})|\,\mathrm{d}s_{n-1}\,\mathrm{d}s_n \\
&\vdots \\
&\le C^n \int_{0<s_1<s_2<\cdots<s_n<t} |x(s_1) - \tilde{x}(s_1)|\,\mathrm{d}s_1\,\mathrm{d}s_2 \ldots \mathrm{d}s_n \\
&\le \frac{C^n}{n!} \sup_{s\in(-T,T)} |x(s) - \tilde{x}(s)|.
\end{aligned}$$

Taking a supremum over $t \in (-T,T)$, we obtain

$$\sup_{t\in(-T,T)} |x(t) - \tilde{x}(t)| \le \frac{C^n}{n!} \sup_{s\in(-T,T)} |x(s) - \tilde{x}(s)|$$

for all n. As the LHS and RHS are finite since x and $\tilde{x}$ are in $C([-T,T] \to X)$, we send $n \to \infty$ to conclude that $x(t) \equiv \tilde{x}(t)$.

Lastly, we claim that the solution depends continuously upon the initial data. Suppose $x(t)$ and $\tilde{x}(t)$ are both solutions to (A.1) in $C([-T,T] \to X)$

with different initial data. Arguing as before, we estimate

$$\begin{aligned}|x(t)-\tilde{x}(t)| &\leq |x(0)-\tilde{x}(0)| + C\int_0^t |x(s_{n-1})-\tilde{x}(s_{n-1})|\,\mathrm{d}s_{n-1}\\ &\vdots\\ &\leq |x(0)-\tilde{x}(0)|\left[1+Ct+\frac{C^2t^2}{2!}+\cdots+\frac{C^nt^n}{n!}\right]\\ &\quad+\frac{C^{n+1}t^{n+1}}{(n+1)!}\sup_{s\in(-T,T)}|x(s)-\tilde{x}(s)|.\end{aligned}$$

The supremum is finite and independent of n since x and $\tilde{x}$ are in $C([-T,T]\to X)$. Therefore the last term on the RHS converges to zero, and so sending $n\to\infty$ yields

$$|x(t)-\tilde{x}(t)| \leq |x(0)-\tilde{x}(0)|e^{C|t|}.$$

Taking a supremum over $t\in[-T,T]$, we see that the map $x_0\mapsto x(t)$ is Lipschitz continuous on any bounded time interval. □

Mimicking the proof of continuous dependence, we can also prove the following useful fact:

Lemma A.3 (Grönwall's inequality)**.** *If $f:[0,T]\to[0,\infty)$ is continuous, $a:[0,T]\to[0,\infty)$ is L^1, and*

$$f(t)\leq A+\int_0^t a(s)f(s)\,\mathrm{d}s,$$

then

$$f(t)\leq A\exp\left\{\int_0^t a(s)\,\mathrm{d}s\right\}.$$

Many authors choose to prove Lemma A.3 first, and then cite it in the proof of Theorem A.2.

Notice that the proof actually shows that the **data-to-solution map** $x_0\mapsto x(t)$ is a Lipschitz function from X into $C([-T,T]\to X)$, and that the Lipschitz constant is bounded by e^{CT}. In fact, it follows that for fixed t the map $x_0\mapsto x(t)$ is a bi-Lipschitz homeomorphism, because we can reconstruct $x(0)$ from $x(t)$ by solving the ODE backwards in time and citing uniqueness. The Lipschitz continuity here matches the Lipschitz continuity of f, and in general we cannot do better.

Another common proof of Theorem A.2 is based on contraction mapping. However, this only proves the result for $T>0$ sufficiently small. The full statement of Theorem A.2 requires our iteration argument.

Next, we would like to extend our existence result to include equations where f is not globally Lipschitz, but instead is smooth. Note that f being smooth does not imply that there are global solutions:

Example A.4. The equation

$$\dot{x} = x^2, \qquad x(0) = 1$$

has solution

$$x(t) = \frac{1}{1-t},$$

which blows up at $t = 1$.

Smoothness does guarantee local solutions however:

Theorem A.5. *If $f : \mathbb{R} \times X \to X$ is continuous and is C^1 in x, then given $x_0 \in X$ there exists $T > 0$ and a unique solution $x : (-T, T) \to X$ in $C([-T, T] \to X)$ to the IVP* (A.1) *that depends continuously upon the initial data.*

Proof. As f' is continuous, there exists $\delta > 0$ and $A > 0$ such that $|t|+|x-x_0| < \delta$ implies $\|f'(t, x)\| \leq A$. In particular, f is Lipschitz on the set $|t|+|x-x_0| < \delta$.

Let $\psi : [0, \infty) \to \mathbb{R}$ be a smooth cutoff function so that $\psi(r) \equiv 1$ for $r \in [0, \frac{\delta}{2}]$ and $\psi(r) \equiv 0$ for $r \geq \delta$. We can now apply the Picard–Lindelöf theorem (Theorem A.2) to

$$\dot{x} = f(t, x)\psi(t)\psi(|x - x_0|), \qquad x(0) = x_0.$$

Lastly, we choose $T > 0$ small enough to stop the solution from noticing the change in the RHS. □

Lastly, we note that solutions $x(t)$ should always be defined on open intervals, since given one defined on a closed interval we can always extend it a bit further.

Corollary A.6 (Blowup criterion)**.** *Suppose $f : \mathbb{R} \times X \to X$ is continuous and is C^1 in x, and fix $x_0 \in X$. Then there exists a maximal interval of existence (T_-, T_+) for some $-\infty \leq T_- < 0 < T_+ \leq \infty$ and a unique solution $x : (-T_-, T_+) \to X$ to the IVP* (A.1)*. Moreover, if T_+ is finite then $|x(t)| \to \infty$ as $t \uparrow T_+$, and similarly for T_-.*

Proof. We define the maximal interval of existence to be the union of all open intervals containing t_0 on which a solution $x(t)$ exists. By Theorem A.5, this is an open and connected set and hence is indeed an interval (T_-, T_+). We may then glue all of these solutions together by uniqueness to obtain a solution $u : (T_-, T_+) \to X$.

Suppose for a contradiction that $T_+ < +\infty$ and $|x(t)| \not\to \infty$ as $t \uparrow T_+$. Then there exists an increasing sequence t_n converging to T_+ on which $|x(t)|$ is bounded. Together with $t = T_+$, this is a bounded set on which f' is continuous and hence bounded. Arguing as in Theorem A.5, we may apply Theorem A.2 to construct a solution defined for a short time after $t = T_+$—but this contradicts the maximality of T_+. □

A.2. Alternative approaches to well-posedness

In this section, we display some important arguments which should be included in a study of ODEs. However, they are not strictly necessary for these notes, and so this section can be skipped if desired.

A.2.1. Existence. In the Picard–Lindelöf theorem (Theorem A.2), the data-to-solution map is automatically Lipschitz. This is convenient for nice problems, but it limits the applicability to ODEs where this is true. The following is an alternative method for proving existence based on compactness, and hence only works for $X = \mathbb{R}^d$.

Theorem A.7 (Cauchy–Peano)**.** *Let $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ continuous. Then for every $x_0 \in \mathbb{R}^d$ the IVP* (A.1) *has at least one solution $x : (-T, T) \to \mathbb{R}^d$.*

Proof. We may assume $f(t, x)$ is continuous and bounded, after replacing f by a truncation as in the proof of Theorem A.5. Let $\phi(t, x)$ be a smooth nonnegative function with $\int \phi = 1$, and define $\phi_\epsilon(t, x) := \epsilon^{-d-1}\phi(\frac{t}{\epsilon}, \frac{x}{\epsilon})$. We replace f by the convolution

$$f_\epsilon(t, x) := \iint \phi_\epsilon(s, y) f(t - s, x - y) \, \mathrm{d}y \, \mathrm{d}s.$$

Then f_ϵ is bounded pointwise independently of ϵ, and is Lipschitz for fixed ϵ.

By the Picard–Lindelöf theorem (Theorem A.2), there exists a unique solution $x_\epsilon(t)$ to the modified equation

$$\dot{x} = f_\epsilon(t, x), \qquad x(0) = x_0.$$

Notice that

$$x_\epsilon(t) = x_0 + \int_0^t f_\epsilon(s, x_\epsilon(s)) \, \mathrm{d}s \tag{A.4}$$

is Lipschitz uniformly in ϵ, since

$$|x_\epsilon(t) - x_\epsilon(s)| \le \int_s^t |f_\epsilon(\tau, x_\epsilon(\tau))| \, \mathrm{d}\tau \le |t - s| \|f\|_{L^\infty}.$$

Therefore $x_\epsilon : [-1, 1] \to \mathbb{R}^d$ for $\epsilon \in (0, 1]$ form a bounded (take $s = 0$ above) and equicontinuous set of functions. By the Arzelà–Ascoli theorem, there exists a sequence $\epsilon_n \to 0$ such that $x_{\epsilon_n}(t)$ converges uniformly on $[-1, 1]$ to some $x(t)$. (This step requires Euclidean space $\mathbb{R}^d$ instead of a general Banach space X, but still works if the image of f is precompact.) Sending $\epsilon_n \to 0$ in the integral equation (A.4), we get

$$x(t) = x_0 + \int_0^t f(s, x(s)) \, \mathrm{d}s.$$

Therefore $x(t)$ solves the IVP by Lemma A.1. We then pick $T > 0$ small so that $x(t)$ solves the original IVP. □

A.2.2. Uniqueness. Note that the statement of Theorem A.7 provides existence, but not uniqueness. This is good for problems where solutions are not unique. For example, the IVP

$$\dot{x} = 2\sqrt{|x|}, \qquad x(0) = 0$$

has solutions $x(t) \equiv 0$ and $x(t) = t^2$.

However, for all other IVPs we would like to prove that solutions are unique. We will now present various arguments for uniqueness.

Our first tool is Grönwall's inequality:

Proposition A.8 (Uniqueness by Grönwall)**.** *Suppose $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ is Lipschitz in x. Then for every $x_0 \in X$ the IVP* (A.1) *has at most one solution.*

Proof. Suppose $x(t)$ and $\tilde{x}(t)$ both solve the IVP (A.1). As f is Lipschitz,

$$|x(t) - \tilde{x}(t)| \leq \int_0^t C|x(s) - \tilde{x}(s)| \, \mathrm{d}s,$$

and so by Grönwall's inequality (Lemma A.3) we have $x(t) \equiv \tilde{x}(t)$. □

Second, we have a monotonicity argument:

Proposition A.9 (Uniqueness by monotonicity)**.** *Suppose $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ satisfies*

$$(x - y) \cdot [f(t, x) - f(t, y)] \leq 0. \tag{A.5}$$

Then for every $x_0 \in X$ the IVP (A.1) *has at most one solution.*

When $d = 1$, the condition (A.5) says that f is decreasing.

Proof. Given two solutions $x(t)$ and $\tilde{x}(t)$ with the same initial data, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}[x(t) - \tilde{x}(t)]^2 = 2[x(t) - \tilde{x}(t)] \cdot [f(t, x(t)) - f(t, \tilde{x}(t))] \leq 0.$$

So by Grönwall's inequality (Lemma A.3) we have $x(t) \equiv \tilde{x}(t)$. □

Note that the proof still applies even if we only have

$$(x - y) \cdot [f(t, x) - f(t, y)] \leq C|x - y|^2.$$

Third, we have a barrier argument:

Proposition A.10 (Uniqueness by barrier)**.** *Suppose $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ satisfies*

$$|f(t, x) - f(t, y)| \leq |x - y| \log \tfrac{1}{|x-y|} \quad \text{for } |x - y| \leq \tfrac{1}{2}. \tag{A.6}$$

Then for every $x_0 \in X$ the IVP (A.1) *has at most one solution.*

Note that the assumption (A.6) on f is slightly weaker than Lipschitz continuity.

Proof. Fix two solutions $x(t)$ and $\tilde{x}(t)$ with the same initial data. We may assume that $|x(t) - \tilde{x}(t)| \leq \frac{1}{2}$ by first restricting our attention to sufficiently small time intervals, and then patching these intervals together. This allows us to estimate

$$|x(t) - \tilde{x}(t)| \leq \int_0^t |x(s) - \tilde{x}(s)| \log \tfrac{1}{|x(s)-\tilde{x}(s)|} \, \mathrm{d}s.$$

Fix $A > 0$, and define the "barrier" $b(t) = \exp\{-Ae^{-t}\}$, which solves the equation

$$\dot{b} = b \log \tfrac{1}{b}, \qquad b(0) = e^{-A}. \tag{A.7}$$

We claim that $|x(t) - \tilde{x}(t)| \leq b(t)$. Suppose this is false. It is true at $t = 0$, and so by continuity there exists a minimal time $t_0 > 0$ where it fails, i.e.

$$|x(t) - \tilde{x}(t)| < b(t) \quad \text{for all } t \in [0, t_0), \qquad |x(t_0) - \tilde{x}(t_0)| = b(t_0).$$

Then by continuity,

$$|x(t_0) - \tilde{x}(t_0)| \leq \int_0^{t_0} |x(s) - \tilde{x}(s)| \log \tfrac{1}{|x(s)-\tilde{x}(s)|} \, \mathrm{d}s < \int_0^{t_0} b \log \tfrac{1}{b} \, \mathrm{d}s = b(t_0),$$

which contracts the choice of t_0.

Together, we have shown that for any $A > 0$ we have $|x(t) - \tilde{x}(t)| \leq b(t)$. Sending $A \to \infty$, we conclude that $|x(t) - \tilde{x}(t)| \leq 0$ and hence $x(t) \equiv \tilde{x}(t)$. □

The assumption (A.6) we must place on f is dictated by the differential equation (A.7) for the barrier b. All we need to make this argument work though is that the differential equation $\dot{b} = g(b)$ satisfies $\int_0^\epsilon \frac{1}{g(b)} \, \mathrm{d}b = \infty$.

Fourth, we have Carleman's approach:

Proposition A.11 (Uniqueness by Carleman estimate)**.** *Suppose that $f : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ is continuous and*

$$|f(t, x) - f(t, y)| \leq C|x - y| \quad \textit{for all } x, y \in \mathbb{R}.$$

Then for every $x_0 \in X$ the IVP (A.1) *has at most one solution.*

We begin with an inequality:

Lemma A.12 (A Carleman estimate)**.** *If $w : \mathbb{R} \to \mathbb{R}$ is C^1 and compactly supported, then*

$$\int e^{2\lambda t} \dot{w}^2 \, dt \geq \int \lambda^2 e^{2\lambda t} w^2 \, dt \quad \textit{for all } \lambda \in \mathbb{R}. \tag{A.8}$$

Proof. We write

$$\begin{aligned} \int e^{2\lambda t} \dot{w}^2 \, \mathrm{d}t &= \int \left[\frac{\mathrm{d}}{\mathrm{d}t}(e^{\lambda t} w) - \lambda e^{\lambda t} w \right]^2 \mathrm{d}t \\ &= \int \left[\left(\frac{\mathrm{d}}{\mathrm{d}t}(e^{\lambda t} w) \right)^2 - 2\lambda (e^{\lambda t} w) \frac{\mathrm{d}}{\mathrm{d}t}(e^{\lambda t} w) + \lambda^2 e^{2\lambda t} w^2 \right] \mathrm{d}t. \end{aligned}$$

The first term on the RHS is nonnegative, and so we can drop it to obtain an inequality. The second term is equal to $-\lambda\frac{\mathrm{d}}{\mathrm{d}t}[(e^{\lambda t}w)^2]$, which integrates to zero since w has compact support. The inequality (A.8) follows. □

Proof of Proposition A.11. Let $x(t)$ and $\tilde{x}(t)$ be two solutions to the IVP (A.1) with the same initial data. We may assume that x and $\tilde{x}$ disagree in the future after substituting $t \mapsto -t$ if necessary. We may also modify $\tilde{x}$ so that $\tilde{x}(t) \equiv x(t)$ for all $t \leq 0$.

Fix $\delta > 0$, and let $\chi : \mathbb{R} \to \mathbb{R}$ be a smooth function so that $\chi(t) \equiv 1$ for $t \leq \delta$ and $\chi(t) \equiv 0$ for $t \geq 2\delta$. Then the weight $w(t) = \chi(t)[\tilde{x}(t) - x(t)]$ is C^1 and compactly supported, and so the Carleman estimate (A.8) yields

$$\begin{aligned}
&\lambda^2 \int e^{2\lambda t}\chi(t)^2[\tilde{x}(t) - x(t)]^2 \,\mathrm{d}t \\
&\leq \int e^{2\lambda t}\big[\dot{\chi}(\tilde{x} - x) + \chi(f(t,\tilde{x}(t)) - f(t,x(t)))\big]^2 \,\mathrm{d}t \\
&\leq C^2 \int e^{2\lambda t}\chi(t)^2|\tilde{x}(t) - x(t)|^2 \,\mathrm{d}t \\
&\quad + \int e^{2\lambda t}\dot{\chi}(t)^2|\tilde{x}(t) - x(t)|^2 \,\mathrm{d}t + 2C \int e^{2\lambda t}|\dot{\chi}(t)\chi(t)||\tilde{x}(t) - x(t)|^2 \,\mathrm{d}t.
\end{aligned}$$

Let $A = \sup\{|\dot{\chi}(t)| : t \in \mathbb{R}\}$, and note that $A \geq c\delta^{-1}$ for some $c > 0$ since χ decreases by 1 over an interval of length δ. Then

$$\begin{aligned}
&\lambda^2 \int e^{2\lambda t}\chi(t)^2[\tilde{x}(t) - x(t)]^2 \,\mathrm{d}t \\
&\leq C^2 \int e^{2\lambda t}\chi(t)^2|\tilde{x}(t) - x(t)|^2 \,\mathrm{d}t + (A^2 + 2AC)\int_\delta^{2\delta} e^{2\lambda t}2(|\tilde{x}|^2 + |x|^2) \,\mathrm{d}t.
\end{aligned}$$

The second term on the RHS is bounded by a constant times $e^{2\delta\lambda}$. Therefore, for all $\lambda \leq -1$ sufficiently large we have

$$\frac{\lambda^2}{4} \int e^{2\lambda t}\chi(t)^2[\tilde{x}(t) - x(t)]^2 \,\mathrm{d}t \leq C' e^{-2\delta|\lambda|}$$

for some constant C'. This implies that the LHS is zero. Indeed, if $|\tilde{x}(t) - x(t)| \not\equiv 0$ on $(0, \delta)$, then there is a time $t_0 \in (0, \delta)$ such that

$$\frac{\lambda^2}{4} \int e^{2\lambda t}\chi(t)^2[\tilde{x}(t) - x(t)]^2 \,\mathrm{d}t \geq c\lambda^2 e^{-2t_0\lambda}$$

for some $c > 0$, and the RHS cannot bounded by $e^{-2\delta|\lambda|}$ for all $\lambda \leq -1$ large.

As $\delta > 0$ was arbitrary, we conclude that $x(t) \equiv \tilde{x}(t)$. □

In other applications, the parameter δ often needs to be fixed small for some other reason. To accommodate this, we can pick $t = 0$ to be the first time after which $x(t)$ and $\tilde{x}(t)$ disagree.

One application of Carleman's argument is Laplace's equation $\Delta u = 0$ in $\mathbb{R}^d$. For $d = 2$, uniqueness can be easily proved by methods of complex analysis. These methods do not carry over at all to $d \geq 3$ however, but Carleman's argument does.

A.2.3. Continuous dependence. Once we have proved existence and uniqueness, we can sometimes recover continuous dependence via a compactness argument.

Proposition A.13. *Let $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ be continuous, and suppose all solutions to the IVP* (A.1) *exist, are bounded, and are unique on some interval $[0, T]$. Then the IVP* (A.1) *is well-posed.*

Proof. It only remains to show continuous dependence. Consider a convergent sequence of initial data $\xi_n \to \xi$. We want to show that the corresponding solutions $x_n(t) := x(t; \xi_n)$ converge uniformly to $x(t; \xi)$.

Observe that the sequence $\{x_n(t)\}$ is equicontinuous on $[0, T]$, since

$$|\dot{x}_n(t)| \leq |f(t, x_n(t))|;$$

the input $x_n(t)$ is bounded uniformly in $n \in \mathbb{N}$ and $t \in [0, T]$ and f is continuous, and so the RHS is also uniformly bounded. Fix an arbitrary subsequence of $\{x_n(t)\}$. By the Arzelà–Ascoli theorem, there exists a further subsequence which converges uniformly. The uniform convergence implies that the limit $y(t)$ will solve the integral equation

$$y(t) = \xi + \int_0^t f(s, y(s)) \, \mathrm{d}s,$$

and hence will solve the IVP (A.1) with initial data ξ by Lemma A.1. Solutions are unique by premise, and so the limit function must be $x(t; \xi)$.

As the initial subsequence was arbitrary, we conclude that the entire sequence $x_n(t)$ converges to $x(t; \xi)$. □

A.3. Smooth dependence upon initial data

If f is C^1 in x, then the following proposition shows that the data-to-solution map is also C^1. This will be useful because we will want to be able to compute volumes in phase space.

Proposition A.14. *Let $f : \mathbb{R} \times X \to X$ be continuous, and be Lipschitz and C^1 in x, and let $x(t; x_0)$ denote the unique solution to the IVP* (A.1). *Then $x(t; x_0)$ is a C^1 function of x_0, and the derivative $V(t; x_0) = \partial_{x_0} x(t)$ is the unique solution to*

$$\dot{V}(t) = f'(t, x(t))V(t), \qquad V(0) = Id_X.$$

Proof. The Picard–Lindelöf theorem (Theorem A.2) applies to V equation, because the RHS is continuous in times and linear in V.

Let $E_h(t)$ denote the quantity

$$\sup_{|\eta|\le h}\left|\frac{f(t,x(t;x_0+\eta))-f(t,x(t;x_0))}{h}-f'(t,x(t;x_0))\frac{x(t;x_0+\eta)-x(t;x_0)}{h}\right|.$$

Observe that $|E_h(t)|\lesssim 1$ uniformly on $[0,T]$, because f and $x_0\mapsto x(t;x_0)$ are both Lipschitz. We also know that $E_h(t)\to 0$ as $h\downarrow 0$ for each t, because $|x(t;x_0+\eta)-x(t;\eta)|\lesssim e^{C|t|}|\eta|$ and f is differentiable at x_0.

Now, for $\eta\neq 0$ we have

$$\begin{aligned}&\left|x(t;x_0+\eta)-x(t;x_0)-\left(\eta+\int_0^t f'(s,x(s))[x(t;x_0+\eta)-x(t;x_0)]\,\mathrm{d}s\right)\right|\\&\le|\eta|\int_0^T E_{|\eta|}(s)\,\mathrm{d}s.\end{aligned}$$

This is the integral equation for

$$V(t)\eta=\eta+\int_0^t f'(s,x(s))V(s)\eta\,\mathrm{d}s.$$

Thus

$$\begin{aligned}&|x(t;x_0+\eta)-x(t;x_0)-V(t)\eta|\\&\le|\eta|\int_0^T E_{|\eta|}(s)\,\mathrm{d}s+\int_0^T\|f'(s,x(s))\|_{\mathrm{op}}|x(s;x_0+\eta)-x(s;x_0)-V(s)\eta|\,\mathrm{d}s.\end{aligned}$$

Note that $\|f'(s,x(s))\|_{\mathrm{op}}$ is bounded uniformly for $s\in[0,T]$. So by Grönwall's inequality (Lemma A.3),

$$|x(t;x_0+\eta)-x(t;x_0)-V(t)\eta|\le|\eta|e^{\sup_s\|f'\|_{\mathrm{op}}}\int_0^T E_h(s)\,\mathrm{d}s.$$

Taking a supremum in η, we obtain

$$\sup_{|\eta|\le h}|x(t;x_0+\eta)-x(t;x_0)-V(t)\eta|\le he^{\sup_s\|f'\|_{\mathrm{op}}}\int_0^T E_h(s)\,\mathrm{d}s.$$

The integral on the RHS converges to zero as $h\downarrow 0$ by the dominated convergence theorem. (For infinite dimensional X, these are Riemann integrals, and so we replace the dominated convergence theorem by the Arzelà convergence theorem—a fact surprisingly more difficult to prove within the context of Riemann integration.) Therefore $\frac{\partial x(t)}{\partial x_0}$ exists and is equal to $V(t)$.

It only remains to show that $x_0 \mapsto V(t; x_0)$ is continuous. We estimate

$$\begin{aligned}
&\|V(t, x_0 + \eta) - V(t; x_0)\| \\
&\leq \int_0^t \|f'(s, x(s; x_0 + \eta))V(s; x_0 + \eta) - f'(s, x(s; x_0))V(s; x_0)\| \, \mathrm{d}s \\
&\leq \int_0^t \|f'(s, x(s))\|_{\mathrm{op}} \|V(s; x_0 + \eta) - V(s; x_0)\| \, \mathrm{d}s \\
&\quad + \int_0^T \|f'(s, x(s; x_0 + \eta)) - f'(s, x(s; x_0))\| \|V(s; x_0 + \eta)\| \, \mathrm{d}s.
\end{aligned}$$

For the second integral on the RHS, we have

$$\|f'(s, x(s; x_0 + \eta)) - f'(s, x(s; x_0))\| \to 0$$

for each s, since

$$|x(s; x_0 + \eta) - x(s; x_0)| \leq |\eta| \exp\left\{\|f\|_{\mathrm{Lip}} T\right\}.$$

Also, the factor $\|V(s; x_0 + \eta)\|$ is bounded, since by the differential equation we have

$$\|V(s; x_0 + \eta)\| \leq 1 \cdot \exp\left\{\|f\|_{\mathrm{Lip}} T\right\}.$$

Therefore, an application of Grönwall's inequality (Lemma A.3) finishes the proof. □

We can extend this to include both higher degrees of regularity and dependence on parameters:

Corollary A.15. *If $f : \mathbb{R}_t \times \mathbb{R}^d_x \times \mathbb{R}^k_\mu \to \mathbb{R}^d$ is C^r in (x, μ) and Lipschitz in x, then the solution to*

$$\dot{x} = f(t, x(t), \mu), \qquad x(0) = \xi \tag{A.9}$$

is C^r in (ξ, μ).

Proof. We iterate the previous theorem. For example, consider the augmented system

$$\frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} x(t) \\ \frac{\partial x}{\partial \xi}(t) \\ \mu(t) \end{pmatrix} = \begin{pmatrix} f(t, x(t), \mu) \\ \frac{\partial f}{\partial x}(t, x(t), \mu) \frac{\partial x}{\partial \xi}(t) \\ 0 \end{pmatrix} \tag{A.10}$$

with initial data (ξ, Id, μ). Assume that f is C^2 in x and μ. Then the RHS obeys the hypotheses of Proposition A.14, and so we conclude that $x(t)$, $\frac{\partial x}{\partial \xi}(t)$, and $\mu(t)$ are C^1 functions of ξ and μ. □

The augmented system (A.10) is not only useful in proofs, but is also commonly used in numerical integration of the system (A.9) with parameter μ. The time t can also be included in the augmented system, but this yields a weaker smoothness result.

A.4. Vector fields and flows

In differential geometry, vector fields are conflated with first-order differential operators:

$$X(x) = (X^1(x), \dots, X^d(x)) \qquad \longleftrightarrow \qquad X \cdot \nabla = \sum_{i=1}^{d} X^i(x) \frac{\partial}{\partial x^i},$$

where $x = (x^1, \dots, x^d)$. (We intentionally use superscript indices here, because they are useful for bookkeeping. In fact, some authors use Einstein summation notation, where we omit the summation symbol and automatically sum over repeated indices provided that one is superscript and the other is subscript.) This way, first-order differential operators are characterized by being a linear operator that satisfies the product rule.

We define the **commutator** of the vector fields X and Y to be the differential operator

$$[X, Y]f = (XY - YX)f.$$

At first this appears to be a second-order differential operator; however, a computation shows that it is a first order differential operator with coefficients

$$[X, Y]^j = \sum_i \left(X^i \frac{\partial Y^j}{\partial x^i} - Y^i \frac{\partial X^j}{\partial x^i} \right).$$

The commutator satisfies the Jacobi identity

$$[[X, Y], Z] + [[Z, X], Y] + [[Y, Z], X] = 0$$

for all vector fields X, Y, and Z. This can be verified directly, but is not particularly illuminating. Ultimately this is true because operators form an associative algebra, which in turn is true because function composition is always associative. (The Jacobi identity does not exclusively arise from associative algebras however; the cross product also obeys the Jacobi identity, but is not associative.)

A vector field X also has an associated first-order differential equation

$$\dot{x} = X(x). \tag{A.11}$$

Given a vector field X, we define the **flow** $\Phi_X(t) := x(t; \cdot)$ which maps the initial data $\xi \in \mathbb{R}^d$ to the solution $x(t; \xi) \in \mathbb{R}^d$ at time t for the differential equation $\dot{x} = X(x)$.

To leading order, the commutator $[X, Y]$ measures the failure of the flows Φ_X and Φ_Y to commute:

Lemma A.16. *Let X and Y be smooth vector fields on $\mathbb{R}^d$. Then*

$$\big[\Phi(t) \circ \Phi_Y(s) - \Phi_Y(s) \circ \Phi_X(t)\big](\xi) = -st[X, Y](\xi) + \mathcal{O}(s^3 + t^3)$$

as $s, t \to 0$.

Proof. We will Taylor expand the LHS. This is valid because flows are always smooth, and consequently we may also differentiate in any order. We compute

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi_X(t)\circ\Psi_Y(s) = X\circ\Phi_X(t)\circ\Phi_Y(s),$$

and so

$$\big[\Phi_X(t)\circ\Phi_Y(0)\big](\xi) = \xi + tX(\xi) + \tfrac{1}{2}t^2(X\cdot\nabla)X(\xi) + \mathcal{O}(t^3).$$

As $\Phi_Y(0) = Id$, we get the same expression for $\Phi_Y(0)\circ\Phi_X(t)$. In this way, there are no terms involving only t or only s in the Taylor expansion.

Therefore the leading order term in the Taylor expansion is quadratic, with only the st term not necessarily vanishing. We have

$$\left.\frac{\partial^2}{\partial s\,\partial t}\right|_{s,t=0}\Phi_X(t)\circ\Phi_Y(s) = (Y\cdot\nabla)X,$$
$$\left.\frac{\partial^2}{\partial s\,\partial t}\right|_{s,t=0}\Phi_Y(s)\circ\Phi_X(t) = (X\cdot\nabla)Y.$$

Together, we compute the coefficient of the st term to be

$$\begin{aligned}\left.\frac{\partial^2}{\partial s\,\partial t}\right|_{s,t=0}\big[\Phi_X(t)\circ\Phi_Y(s) - \Phi_Y(s)\circ\Phi_X(t)\big](\xi) &= \big\{(Y\cdot\nabla)X - (X\cdot\nabla)Y\big\}(\xi)\\ &= -[X,Y](\xi)\end{aligned}$$

as desired. □

Integrating in time, we obtain the following important fact:

Theorem A.17. *Let X and Y be smooth vector fields. Then $[X,Y]=0$ if and only if the flows commute:*

$$\Phi_X(t)\circ\Phi_Y(s) = \Phi_Y(s)\circ\Phi_X(t).$$

Proof. We follow the analytic argument from [Arn89, §39.E].

$\Longleftarrow$: This follows immediately from the previous lemma.

$\Longrightarrow$: Fix $s,t\neq 0$. We may assume $s,t>0$ after reversing time if necessary. Fix a positive integer N, and divide the rectangle $[0,t]\times[0,s]$ into an $N\times N$ grid.

Each path from $(0,0)$ to (s,t) along this grid corresponds to a composition of N copies of $\Phi_X(\frac{t}{N})$ and N copies of $\Phi_Y(\frac{s}{N})$ in some order. In particular,

$$\Phi_X(t)\circ\Phi_Y(s) = \Phi_X(\tfrac{t}{N})\circ\cdots\circ\Phi_X(\tfrac{t}{N})\circ\Phi_Y(\tfrac{s}{N})\circ\cdots\circ\Phi_Y(\tfrac{s}{N})$$

and similarly for $\Phi_Y(s)\circ\Phi_X(t)$.

We write the difference $\Phi_X(t)\circ\Phi_Y(s) - \Phi_Y(s)\circ\Phi_X(t)$ as a telescoping sum of N^2 terms, where the summand consists of the difference of two paths that

differ around one grid square. Within the summand, there is a difference of two flows that agree up to one point, differ around a $N^{-1} \times N^{-1}$ box, and then continue as the flows of two possibly different points. Applying the lemma with $[X, Y] = 0$, the difference around one box is

$$\Phi_X(\tfrac{t}{N}) \circ \Phi_Y(\tfrac{s}{N}) - \Phi_Y(\tfrac{s}{N}) \circ \Phi_X(\tfrac{t}{N}) = 0 + \mathcal{O}(\tfrac{|s|^3+|t|^3}{N^3}).$$

After this, the flows can then deviate at most exponentially. Altogether, we estimate the whole sum as

$$\Phi_X(t) \circ \Phi_Y(s) - \Phi_Y(s) \circ \Phi_X(t) = N^2 e^{C(|t|+|s|)} \mathcal{O}(\tfrac{|s|^3+|t|^3}{N^3}).$$

Sending $N \to \infty$, the RHS vanishes. As s, t were arbitrary, we conclude that $\Phi_X(t) \circ \Phi_Y(s) - \Phi_Y(s) \circ \Phi_X(t) \equiv 0$. □

A.5. Behavior away from fixed points

We are ultimately interested in the qualitative characterization of all Hamiltonian flows. First, we will need a general fact about the behavior of solutions away from fixed points.

We say that a diffeomorphism $x = \Psi(y)$ **conjugates** the flow $\dot{x} = X(x)$ into the flow $\dot{y} = Y(y)$ if

$$Y(y) = (\Psi'(y))^{-1}(X \circ \Psi)(y). \tag{A.12}$$

Indeed, under the change of variables $x = \Psi(y)$ we have

$$\dot{x} = \frac{\mathrm{d}}{\mathrm{d}t}\Psi(y) = \Psi'(y)\dot{y} = \Psi'(y)Y(y).$$

On the other hand,

$$\dot{x} = X(x) = (X \circ \Psi)(y),$$

and so rearranging yields the condition (A.12). This is the notion with which we can describe the qualitative behavior of solutions.

Proposition A.18. *If $X(x_0) \neq 0$, then there exists a local diffeomorphism conjugating* (A.11) *to*

$$\dot{y} = \mathbf{e}_1 = (1, 0, \ldots, 0).$$

Proof. We may assume $x_0 = 0$ after translating. First we rotate coordinates so that $X(0) = c\mathbf{e}_1$ with $c > 0$. Let $\Phi_X(t; x) := x(t; \xi)$ denote the flow of the initial data ξ by time t. Define

$$\Psi(y) = \Phi_X(y_1; (0, y_2, \ldots, y_d)).$$

That is, we flow the initial data $(0, y_2, \ldots, y_d)$ by a "time" y_1.

We check that this choice does indeed work. We have

$$\Psi'(y) = \begin{pmatrix} \frac{\partial \Psi_1}{\partial y_1} & \cdots & \frac{\partial \Psi_1}{\partial y_d} \\ \vdots & & \vdots \\ \frac{\partial \Psi_d}{\partial y_1} & \cdots & \frac{\partial \Psi_d}{\partial y_d} \end{pmatrix} = \begin{pmatrix} | & * & \cdots & * \\ X \circ \Psi(y) & \vdots & \ddots & \vdots \\ | & * & \cdots & * \end{pmatrix}, \tag{A.13}$$

where "$*$" denotes an unspecified nonzero entry. In particular,

$$\Psi'(0) = \begin{pmatrix} c & 0 & \dots & 0 \\ 0 & 1 & & \\ \vdots & & \ddots & \\ 0 & & & 1 \end{pmatrix}$$

has determinant $c > 0$ and hence is nonsingular. (The lower right submatrix is the identity because $\Phi_X(0; (0, y_2, \dots, y_d)) = (0, y_2, \dots, y_d)$.) Therefore Ψ is a local diffeomorphism by the inverse function theorem. Also, from (A.13) we see that

$$\Psi'(y)\mathbf{e}_1 = (X \circ \Psi)(y),$$

and so

$$\dot{y} = (\Psi'(y))^{-1}(X \circ \Psi)(y) \equiv \mathbf{e}_1$$

as desired. □

To paraphrase, a nonvanishing vector field X is locally a coordinate vector field $\frac{\partial}{\partial x_1}$ for some choice of coordinates. Unlike general collections of vector fields, coordinate vector fields commute with each other.

Proposition A.19. *If $X_1, \dots, X_n$ smooth vector fields on $\mathbb{R}^d$ that commute and $X_1(x_0), \dots, X_n(x_0) \in \mathbb{R}^d$ are linearly independent, then there exists a local diffeomorphism that conjugates $X_1, \dots, X_n$ into $\mathbf{e}_1, \dots, \mathbf{e}_n$.*

Proof. We may assume $x_0 = 0$ after translating. First, we make a linear change of variables so that $X_1(x_0) = \mathbf{e}_1$, …, $X_n(x_0) = \mathbf{e}_n$, which can be done by linear independence. Let $[\Phi_{X_i}(t)](x) := x_i(t; \xi)$ denote the flow of the initial data ξ under the equation $\dot{x}_i = X_i$ by time t. Define

$$\Psi(y) = \big[\Phi_{X_1}(y_1) \circ \Phi_{X_2}(y_2) \circ \cdots \circ \Phi_{X_n}(y_n)\big](0, \dots, 0, y_{n+1}, \dots, y_d).$$

We have $\Psi'(0) = Id$ as before. As the vector fields commute, so do their flows. Therefore, in computing the ith derivative of Ψ, we may pull the ith flow map Φ_{X_i} out to the front:

$$\frac{\partial \Psi}{\partial y_i} = \frac{\partial}{\partial y_i} \Psi_1 X_i(y_i) \circ [\dots] = X_i \circ \Psi(y) \circ [\dots].$$

The rest of the calculation is the same as in Proposition A.18. □

A.6. Behavior near a fixed point

It remains to describe the behavior of solutions near a point x_0 where $X(x_0) = 0$. Such a point is called a **fixed point** (or **stationary point**, **equilibrium**), because the constant function $x(t) \equiv x_0$ is a solution to $\dot{x} = X(x)$ and hence the flow $\Phi_X(t)$ fixes x_0. The material in this section is not strictly necessary for these notes (and so we omit the proofs); however, it is essential in

a study of ODEs. Nevertheless, the local structure of flows nearby a fixed point is still not fully understood to this day.

A first step is to linearize the vector field $X(x)$:

$$X^i(x) \approx 0 + \sum_{j=1}^{d} \frac{\partial X^i}{\partial x^j}(x_0)x^j.$$

Ideally, we would like to say that the higher order terms that we have neglected are small. A fundamental idea to accomplish this is to write the nonlinear flow as the linear flow plus a perturbation:

Lemma A.20 (Duhamel formula)**.** *Suppose A is a $d\times d$ matrix and $g : \mathbb{R}^d \to \mathbb{R}^d$ is smooth. Then $x \in C^1((-T,T) \to \mathbb{R}^d)$ solves*

$$\dot{x} = Ax + g(x)$$

if and only if $x \in C^0((-T,T) \to \mathbb{R}^d)$ solves

$$x(t) = e^{At}x(0) + \int_0^t e^{A(t-s)}g(x(s))\,\mathrm{d}s. \tag{A.14}$$

In the case $A = 0$, we recover the integral equation (A.2).

Proof. Write $x(t) = e^{At}y(t)$. As A is time-independent, then e^{At} commutes with A and so we may write

$$\dot{y} = -Ay + e^{-At}(Ax + g(x)) = e^{-At}g(x(t)).$$

This is solved if and only if $y(t)$ solves the integral equation

$$y(t) = y(0) + \int_0^t e^{-As}g(x(s))\,\mathrm{d}s.$$

Recalling that $y(t) = e^{-At}x(t)$ and multiplying by e^{At} yields the claim. □

This proof method is called variation of parameters, and it is widely applicable. It is useful even when A is nonlinear, although it is harder.

Even in the case when g is linear, the Duhamel formula (A.14) is nontrivial. Indeed, if we write $g(x) = Bx$ and iterate, then we get

$$\begin{aligned} x(t) = e^{At}x(0) &+ \int_0^t e^{A(t-s)}Be^{As}x(0)\,\mathrm{d}s \\ &+ \iint_{0<s_1<s_2<t} e^{A(t-s_2)}Be^{A(s_2-s_1)}Be^{As_1}x(0)\,\mathrm{d}s_1\,\mathrm{d}s_2 + \dots. \end{aligned}$$

This is the infinite Duhamel expansion, where we sum over the possible histories of $x(t)$. Starting with $x(0)$, we flow by A; to this, we add the flow by A, bump by B, and flow by A; then we add the flow by A, bump by B, flow by A, bump by B, and flow by A; and so on.

Duhamel's formula (A.14) is much more effective than the integral equation (A.2) at solving equations by iteration. Consider

$$\dot{x} = Ax + \epsilon(x), \quad A = \begin{pmatrix} -1 & 0 \\ 0 & -\lambda \end{pmatrix}.$$

In the case $\epsilon = 0$, iterating the integral equation (A.2) yields

$$x(t) = x_0 + (At)x_0 + \tfrac{1}{2}(At)^2 x_0 + \cdots + \tfrac{1}{k!}(At)^k x_0 + \ldots.$$

For $\lambda > 1$ large, we have to go to the term $k \approx \lambda$ before the terms stop growing. On the other hand, e^{At} is very stable, and the Duhamel formula harnesses this.

Back to the behavior near a fixed point. If we make a diffeomorphic change of variables $x = \Psi(y)$, we know from (A.12) that the equation for y is

$$\dot{y} = Y := (\Psi'(y))^{-1}(X \circ \Psi)(y).$$

If Ψ maps 0 to the fixed point x_0, then we obtain

$$\frac{\partial Y^i}{\partial y^j}(0) = [\ldots]X(x_0) + \sum_{k,\ell=1}^{d} \big[\psi'(0)^{-1}\big]^i_k \frac{\partial X^k}{\partial x^\ell}(x_0)\big[\psi'(0)\big]^\ell_j.$$

The first term on the RHS vanishes since $X(x_0) = 0$. Therefore the matrix $\frac{\partial Y^i}{\partial y^j}$ is similar to $\frac{\partial X^i}{\partial x^j}$, because they are conjugated by $\Psi'(0)$. In particular, the Jordan normal form of $\frac{\partial X^i}{\partial x^j}$ (and hence all of its spectral properties) is preserved under this change of variables.

The following fundamental result tells us that often the actual flow is qualitatively similar to the linearized flow:

Theorem A.21 (Hartman–Grobman)**.** *If the matrix $\frac{\partial X^i}{\partial x^j}(x_0)$ has no purely imaginary eigenvalues, then there exists a homeomorphism conjugating the nonlinear flow* (A.11) *to the linear flow*

$$\dot{y} = \sum_{j=1}^{d} \frac{\partial X}{\partial x^j}(x_0) y^j.$$

For a proof, see [KH95]. The assumption of Theorem A.21 is necessary; cf. Example 2.3.

Note that Theorem A.21 only guarantees that the change of variables is homeomorphic, rather than diffeomorphic. It turns out that the change of variables may indeed only be continuous and not differentiable, but the derivative at x_0 must exist and be equal to identity; see [Har60, GHR03] for details. In particular, this justifies that the phase portrait for the nonlinear system must look like the linearized phase portrait near x_0.

However, Theorem A.21 does not tell us what happens to the finer features of the linearized flow. In particular, what happens to the stable and unstable

eigenspaces? The stable and unstable manifold theorems tell us that they are preserved under some additional assumptions. For a general linear system $\dot{x} = Ax$, we define the stable, unstable, and center manifolds:

$$X_s = \bigcup \{\operatorname{span} \ker((A-\lambda)^k) : \operatorname{Re}\lambda < 0\},$$
$$X_u = \bigcup \{\operatorname{span} \ker((A-\lambda)^k) : \operatorname{Re}\lambda > 0\},$$
$$X_c = \bigcup \{\operatorname{span} \ker((A-\lambda)^k) : \operatorname{Re}\lambda = 0\},$$

where λ varies over the eigenvalues of A.

Theorem A.22 (Stable manifold theorem)**.** *Suppose that $f : \mathbb{R}^d \to \mathbb{R}^d$ is smooth and the IVP* (A.1) *has a hyperbolic fixed point at $x = 0$. Then there exists $0 < \delta_0 < \delta_1$ and a smooth function $\psi : \{a : X_s : |a| < \delta_1\} \to X_u$ such that the stable manifold*

$$\mathcal{M} = \{a + \psi(a) : a \in X_s,\ |a| < \delta_1\}$$

satisfies the following:

(a) If $|x_0| < \delta_0$ and $x_0 \in \mathcal{M}$, then the solution $x(t)$ stays in the δ_1 neighborhood:

$$|x(t)| \le \delta_1 \quad \text{for all } t \ge 0,$$

and decays exponentially:

$$|x(t)| \le Ce^{-\sigma t}|x_0| \quad \text{for some } C, \sigma > 0.$$

(b) If $|x_0| < \delta$ and $x_0 \notin \mathcal{M}$, then the solution is ejected from the δ_1 neighborhood:

$$|x(t)| \ge \delta_1 \quad \text{for some } t > 0.$$

See [CL55, §13.4] for a proof. To obtain the statement of the unstable manifold theorem we simply need to reverse time, which swaps $A \mapsto -A$ and $X_s \leftrightarrow X_u$.

The constant σ in part (a) may be strictly smaller than the smallest real part $\inf\{|\operatorname{Re}\lambda| : \operatorname{Re}\lambda < 0\}$, and the constant C must depend on σ. To see this, consider a Jordan block A with eigenvalue $\operatorname{Re}\lambda < 0$ and all ones on the superdiagonal. Then we have

$$e^{At} = e^{\lambda t} \begin{pmatrix} 1 & t & \frac{1}{2}t^2 & \dots \\ 0 & 1 & t & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

Although the factor $e^{\lambda t}$ is exponentially decaying, the matrix is initially growing in t.

A.7. Exercises

A.1. (a) Fix $f : \mathbb{R}\times\mathbb{R}^d \to \mathbb{R}^d$ that is C^1 and consider the initial value problem

$$\dot{x} = f(t, x) \quad \text{with} \quad x(0) = \xi.$$

Suppose that for some ξ_0 this problem admits a (necessarily unique) solution on the interval $[0, T)$. Show that for each $\epsilon > 0$ there is a $\delta > 0$ so that if $|\xi - \xi_0| < \delta$, then the initial value problem admits a solution on the interval $[0, T - \epsilon)$.

(b) Compute the maximal (forward) existence time as a function of the initial data for the problem

$$\dot{x} = \frac{x^2}{1 + y^2x^2}, \quad \dot{y} = 0.$$

Deduce that the existence time may fail to be continuous (in the natural topology on $[0, \infty]$). By part (a), however, it is always lower semi-continuous.

A.2. Suppose that $A(t)$ and $B(t)$ are C^1 square matrices with $\dot{A} = BA$. Show that

$$\frac{\mathrm{d}}{\mathrm{d}t} \det A = \mathrm{tr}(B) \det(A). \tag{A.15}$$

(Hint: : Write the derivative of $\det A$ in terms of the derivatives of its rows and simplify using row operations. Be careful that you do not implicitly assume the eigenvalues are differentiable, which is not true.)

A.3 (Trust singular values, not eigenvalues)**.** Suppose A is a 2×2 matrix with eigenvalues $-\lambda < 0$ and -1, and eigenspaces which form angles $\pm\theta$ with the horizontal axis. Fix $t > 0$ and $\lambda > 1$ sufficiently large. Show that e^{At} has norm $\geq c\theta^{-1}$ for some constant $c > 0$ for all $\theta > 0$ sufficiently small. Even though A has negative eigenvalues, the change of basis matrix makes the norm of e^{At} very large.

A.4. Find an example of 2×2 matrices A and B which both satisfy $X_s = \mathbb{R}^2$ but $A+B$ has $X_u \neq \{0\}$. (Hint: Take A and B to be upper and lower triangular respectively, and consider $\det(A + B)$.) This phenomenon is known as Turning instability, and was introduced in [Tur52].

A.5. The proof of the stable manifold theorem actually shows that $\mathcal{M}$ is a smooth manifold that is tangent to X_s at the origin, following as in the proof of Proposition A.14. With this information in hand, we can derive many properties from the differential equation. For example, consider the system

$$\dot{q} = q - 2pq + 3p^2, \quad \dot{p} = -p + p^2.$$

(Incidentally, this system is Hamiltonian, but this is not important to this method.) On $\mathcal{M}$ we can write $q = \psi(p)$. Taking a time derivative of this equation, match Taylor coefficients using $\psi(0) = 0 = \psi'(0)$ to compute the second-order expansion of ψ at $p = 0$.

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