

Random Mechanical Systems

T. Chumley*, S. Cook† R. Feres‡

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These are lecture notes for a short course to be given at the Houston Summer School on Dynamical Systems, at the University of Houston, May 14-22, 2014. The actual lectures will cover only part of the material contained here but we hope these extended notes will be useful as a reference text on various topics that may be touched on only lightly during the lectures.

1 PRELIMINARIES ON SMOOTH MANIFOLDS AND LIE GROUPS

1.1 GENERALITIES AND NOTATIONS

The mathematical description of classical mechanical systems takes on a particularly clear form when expressed in the language of differential geometry. We review in this section some of the basic concepts, notation, and terminology concerning the local theory of smooth manifolds that will be frequently used in these notes, assuming that the student is already familiar with calculus in \mathbb{R}^n . We begin by recalling the ideas of smooth atlas, tangent vectors, vector fields, and the tangent bundle, and notation pertaining to various kinds of derivatives. Further geometric concepts, such as connections on vector and principal bundles will be introduced later on as needed. Students who have taken a first year graduate course in manifold theory will not see anything new in these geometric digressions. Those who have not will note that the familiar concepts from \mathbb{R}^n mostly extend without a great deal of difficulty to general manifolds. Whether or not you are already familiar with the concepts of this section, we suggest that you quickly skim through it to become acquainted with the notation and terminology, and refer back to it later as needed.

A smooth manifold M of dimension n is a topological space each of whose points admits neighborhoods homeomorphic to open subsets in \mathbb{R}^n , called *coordinate patches*. It is also assumed that on the intersection of two such coordinate patches the two coordinate systems are smoothly compatible, in the sense specified in the following definition. An open cover of M by coordinate patches defines a smooth *atlas* on M , which is the structure we need to develop a differential and integral calculus on M . We will keep the formal definitions to a minimum. For further elaboration we recommend [5].

Definition 1.1 (Smooth manifolds). An n -dimensional *smooth manifold* M is a Hausdorff, paracompact topological space (i.e., a topological space in which every open cover admits a

*Department of Mathematics, Iowa State University, Ames, IA 50011

†Department of Mathematics and Statistics, Swarthmore College, College Ave, Swarthmore PA 19081

‡Department of Mathematics, Washington University, Campus Box 1146, St. Louis, MO 63130

locally finite open refinement) equipped with an *atlas* of coordinate charts $\{\phi_\alpha : U_\alpha \rightarrow V_\alpha\}_{\alpha \in \mathcal{A}}$ where, for each α , V_α is an open subset of \mathbb{R}^n , ϕ_α is a homeomorphism, $\{U_\alpha\}_{\alpha \in \mathcal{A}}$ is an open cover of M , and

$$\phi_\beta \circ \phi_\alpha^{-1}|_{\phi_\alpha(U_\alpha \cap U_\beta)} : \phi_\alpha(U_\alpha \cap U_\beta) \rightarrow \phi_\beta(U_\alpha \cap U_\beta)$$

is a diffeomorphism for each pair $\alpha, \beta \in \mathcal{A}$ for which $U_\alpha \cap U_\beta$ is not empty.

The ring of smooth functions on M , denoted $C^\infty(M)$, consists of continuous functions f such that $f \circ \phi_\alpha^{-1}$ is smooth on V_α , for each α . Differentiability of maps, vector fields and other kinds of tensor fields is similarly defined by requiring that local expressions of those objects in the coordinates associated to the ϕ_α be differentiable.

We now introduce the concept of tangent vectors. The main point to bear in mind is that, in the absence of an affine space structure on a general manifold M , we cannot define a vector as the difference of two points, but we can define the notion of directional derivative as we show below. Tangent vectors at a point q are then defined by their identification with directional derivatives along directions defined by equivalent classes of smooth paths that are in tangential contact at q . The details are as follows. For any given point q in M , an equivalence relation can be defined on the set of differentiable curves through q as follows. Two paths $\gamma_i : (-a_i, a_i) \rightarrow M$, $i = 1, 2$, such that $\gamma_i(0) = q$, are said to be equivalent at q if for any smooth function f on M

$$(f \circ \gamma_1)'(0) = (f \circ \gamma_2)'(0).$$

Equivalence classes, $v = [\gamma]_q$, are called *tangent vectors* to M at q . If $M = \mathbb{R}^n$, there is a natural bijection between vectors v (elements of the vector space \mathbb{R}^n) and classes of differentiable curves: $v \mapsto [t \mapsto q + tv]_q$, but the given definition makes sense even when M is not a vector space. The set of all tangent vectors at q is denoted $T_q M$, and is called the *tangent space* to M at q . A tangent vector $v = [\gamma]_q$ defines a differentiation on $C^\infty(M)$ by

$$(1.1) \quad v f := (f \circ \gamma)'(0)$$

which does not depend on the representative curve γ . We call $v f$ the *directional derivative* of f along v at q . Very often we employ the following expression: Let γ be a path *representing* the vector $v \in T_q M$. By this we mean that $\gamma : (-a, a) \rightarrow M$ is a smooth path such that $\gamma(0) = q$ and $\gamma'(0) = v$, the latter being defined by the identity 1.1 for every smooth function f .

Given a differentiable map between manifolds, $F : M \rightarrow N$, and a point q in M , the *derivative map* (or the *Jacobian map*, or the *differential of F at q*) is a linear map dF_q from $T_q M$ to $T_{F(q)} N$ defined by $dF_q[\gamma]_q = [F \circ \gamma]_{F(q)}$. In terms of the directional derivative v we can write

$$(dF_q v) f = v(f \circ F)$$

for each $f \in C^\infty(N)$. An immediate consequence of this definition is the chain rule:

$$d(F \circ G)_q = dF_{G(q)} \circ dG_q.$$

Let v be a tangent vector to M at q and $\phi : U \rightarrow V \subset \mathbb{R}^n$ a local coordinate system on a neighborhood U of q . We write $\phi = (x_1, \dots, x_n)$. Let $\bar{v} = d\phi_p v$ be the image of v in the tangent

space of \mathbb{R}^n at $\phi(q)$. Regarding \bar{v} as a derivative on functions on \mathbb{R}^n , it is not difficult to conclude from the definitions that there are numbers a_j such that

$$\bar{v}f = \sum_{j=1}^n a_j \frac{\partial f}{\partial x_j}(\phi(q)).$$

The partial derivatives $\{\partial_{x_1}, \dots, \partial_{x_n}\}$ (evaluated at $\phi(q)$) constitute a basis of $T_{\phi(q)}\mathbb{R}^n$. (We may use ∂_{x_j} or $\partial/\partial x_j$ interchangeably.) We also use these partial derivatives to denote the corresponding basis of T_qM obtained under the isomorphism $(d\phi_q)^{-1}$.

Now let F be a differentiable map from M to N . The *Jacobian matrix* of dF_q is the matrix of the linear map in terms of the coordinate basis vectors around q and $F(q)$. A simple calculation shows that it has the familiar form we learn in multivariable calculus. We typically express a vector $v \in T_pM$ in a coordinate system $\phi = (x_1, \dots, x_n)$ by

$$v = \sum_{j=1}^n a_j \partial_{x_j}.$$

The *tangent bundle* TM is defined as the disjoint union of the T_qM for all q . Elements of TM are usually written as pairs (q, v) , where q lies in M and v belongs to T_qM . We often omit q and let v represent all by itself an element of TM . Let $\pi : TM \rightarrow M$ denote the *base point* map, which assigns to (q, v) in TM the point q . Typically, we simply write $\pi(v) = q$. For each coordinate chart (U, ϕ) in a smooth atlas of M we define $(\bar{U}, \bar{\phi})$ as follows: $\bar{U} = \pi^{-1}(U)$, and $\bar{\phi} : \bar{U} \rightarrow \mathbb{R}^n \times \mathbb{R}^n$ is such that

$$(q, v) \in TM \mapsto \bar{\phi}(q, v) = (\phi(q), d\phi_q v) \in \mathbb{R}^n \times \mathbb{R}^n.$$

We are here identifying $T_{\phi(q)}\mathbb{R}^n$ with \mathbb{R}^n . If $\phi = (x_1, \dots, x_n)$, a common notation in physics that we will often adopt is

$$\bar{\phi} = (x_1, \dots, x_n, \dot{x}_1, \dots, \dot{x}_n).$$

Thus from the coordinates x_i on $U \subset M$ we obtain coordinates x_i, \dot{x}_i on \bar{U} so that

$$\bar{\phi}(q, v) = \left(x_1(q), \dots, x_n(q), \sum_{j=1}^n \dot{x}_j(v) \partial_{x_j} \right).$$

The collection of $\bar{\phi}$, for ϕ in a smooth atlas of M constitutes a smooth atlas for TM , thus making TM itself a smooth manifold. This atlas has the special feature that coordinate change maps, which are here maps from $\mathbb{R}^n \times \mathbb{R}^n$ to itself, have the general form $F(x, u) = (f(x, u), A(x)u)$, where $A(x)$ is a linear function of the second factor u . This property characterizes TM as being a *vector bundle*. We will often write q_j for x_j and conflate the point q and its coordinate vector $q = (q_1, \dots, q_n)$. We will find it useful later to introduce the operation $\mathcal{J}_v : T_qM \rightarrow T_{(q,v)}(TM)$ that to each $w \in T_qM$ associates the vector $\left. \frac{d}{ds} \right|_{s=0} (v + sw)$. The latter is a *vertical vector* in the sense that it lies in the kernel of $d\pi_v$. That is, $d\pi_v \circ \mathcal{J}_v = 0$. Note that $\mathcal{J}_v \frac{\partial}{\partial x_j} = \frac{\partial}{\partial \dot{x}_j}$.

1.2 VECTOR FIELDS AND FLOWS

A smooth *vector field* on M is a smooth map $X : M \rightarrow TM$ that associates to each q a tangent vector $X(q) \in T_q M$. We can also define a vector field along a path $\gamma : I \rightarrow M$, where I is an interval in \mathbb{R} , as a map $t \in I \mapsto X(t) \in T_{\gamma(t)} M$. For example, if γ is a differentiable path in M , then the derivative $\gamma'(t)$ is a vector field along γ . We often think of the curve parameter as time, in which case $\gamma'(t)$ is the *velocity* vector field of the path.

The vector field X on M , being a directional derivative at each point, can be regarded as a first order differential operator on $C^\infty(M)$ that sends constant functions to 0. Thus we often think of X as a map $X : C^\infty(M) \rightarrow C^\infty(M)$. This map is an algebraic *derivation* in the sense that for each constant c and smooth functions f, g , the following properties hold:

$$(1.2) \quad Xc = 0, \quad X(f + g) = Xf + Xg, \quad X(fg) = (Xf)g + fXg.$$

Given two smooth vector fields X and Y , their composition XY is then a second order differential operator: $(XY)f = X(Yf)$; thus it makes sense to define

$$[X, Y] = XY - YX,$$

a linear combination of second order operators. It is a simple exercise to show that $[X, Y]$ is, in fact, of first order. Therefore, it is also a vector field. This defines a bilinear operation on smooth vector fields called the *Lie bracket*. These claims are easily verified by expressing the Lie bracket in local coordinates: Given $X = h_1 \partial_{x_1} + \cdots + h_m \partial_{x_m}$, $Y = g_1 \partial_{x_1} + \cdots + g_m \partial_{x_m}$, and a smooth function f ,

$$XYf = \sum_{i,j} \left[h_i \frac{\partial g_j}{\partial x_i} \frac{\partial f}{\partial x_j} + h_i g_j \frac{\partial^2 f}{\partial x_i \partial x_j} \right],$$

and

$$[X, Y]f = \sum_{i,j} \left[h_i \frac{\partial g_j}{\partial x_i} - g_i \frac{\partial h_j}{\partial x_i} \right] \frac{\partial f}{\partial x_j}.$$

Exercise 1.1 (The Lie bracket). Verify the claim that if X, Y are smooth vector fields on M , then $[X, Y]$ is also a smooth vector field. Note: it suffices to check that the above three properties 1.2 characterizing a derivation on $C^\infty(M)$ are satisfied. The Lie bracket turns the vector space of vector fields into a non-associative algebra. Show that this algebra of vector fields satisfies the following properties, where X, Y, Z are vector fields, a, b are real numbers, and f is a smooth function:

1. Linearity: $[aX + bY, Z] = a[X, Z] + b[Y, Z]$;
2. Skew-symmetry: $[X, Y] = -[Y, X]$;
3. Jacobi identity: $[X, [Y, Z]] = [[X, Y], Z] + [Y, [X, Z]]$;
4. Leibnitz property: $[X, fY] = (Xf)Y + f[X, Y]$;

A vector space with a bilinear operation satisfying the properties (2) and (3) stated in Exercise 1.1 is called a *Lie algebra*. The *Lie derivative* of a vector field Y along another vector field X is

$$\mathcal{L}_X Y = [X, Y].$$

Note that the Jacobi identity amounts to a product rule for the Lie bracket:

$$\mathcal{L}_X[Y, Z] = [\mathcal{L}_X Y, Z] + [X, \mathcal{L}_X Z].$$

A vector field X on M can also be regarded as a differential equation on M . A smooth path $\gamma(t)$ is said to be an *integral curve* of X if it satisfies the equation

$$\gamma'(t) = X(\gamma(t))$$

for each t . Here $X(\gamma(t)) = X_{\gamma(t)}$ indicates the tangent vector at $\gamma(t)$. This means that if f is any smooth function, then

$$\frac{d}{dt}f(\gamma(t)) = (Xf)(\gamma(t))$$

for each t . From the general theory of ordinary differential equations, integral curves through a point $q = \gamma(0)$ exist, at least for sufficiently small values of t , and are unique (over an interval of t where it exists). If such solutions exist for all $t \in \mathbb{R}$ we say that X is a *complete* vector field. This is the case, for example, when X has compact support, but it can be true much more generally. When X is complete, we have a smooth map $\Phi: \mathbb{R} \times M \rightarrow M$ such that, for each $q \in M$, the path $\gamma(t) = \Phi(t, q)$ is the unique integral curve of X such that $\gamma(0) = q$. It can be shown that $\Phi_t := \Phi(t, \cdot)$ is a diffeomorphism of M to itself and that the following *flow property* holds:

$$\Phi_{t+s} = \Phi_t \circ \Phi_s.$$

Thus $t \mapsto \Phi_t$ is a homomorphism from the additive group \mathbb{R} to the group of diffeomorphism of M . We refer to Φ as the *flow* of X . When X is not complete, we can still define a pseudo-group of local diffeomorphisms.

Exercise 1.2. Show that Lie derivative satisfies

$$\mathcal{L}_X Y = - \left. \frac{d}{dt} \right|_{t=0} \Phi_{t*} Y,$$

where $\Phi_{t*} Y$ is the *push-forward* of Y under the local flow of X , defined by

$$(\Phi_{t*} Y)_q := (d\Phi_t)_{\Phi_{-t}(q)} Y(\Phi_{-t}(q)).$$

A similar characterization of $\mathcal{L}_X Y$ exists using an appropriately defined *pull-back* operation.

We illustrate these ideas with linear vector fields on \mathbb{R}^n . Let $M(n, \mathbb{R})$ denote the vector space of all n -by- n real matrices. To $A = (a_{ij}) \in M(n, \mathbb{R})$, we associate the vector field

$$X_x^A := \sum_{ij} a_{ij} x_{ij} \frac{\partial}{\partial x_j}.$$

Alternatively, we write $X^A(x) = A^\dagger x$. To this vector field is associated the system of linear differential equations with constant coefficients $\dot{x} = A^\dagger x$. We know from the general theory of differential equations that X^A is a complete vector field and its flow is obtained by matrix exponentiation:

$$\Phi_t(x) = \exp(tA^\dagger)x.$$

Exercise 1.3. Show that the flow of diffeomorphisms on \mathbb{R}^2 generated by the vector field X^A , where Let $A = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ is given by

$$\Phi_t(x) = \begin{pmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

Exercise 1.4. Show that the Lie bracket of the linear vector fields X^A and X^B is given by

$$[X^A, X^B] = X^{[A, B]}$$

where $[A, B] = AB - BA$. (This identity is the main reason we chose to define X^A using the transpose of A .)

Exercise 1.5. Let Φ_t be the flow associated to a vector field X on a manifold M and f any smooth function on M . Show that

$$\frac{d}{dt} f(\Phi_t(q)) = (Xf)(\Phi_t(q)).$$

Exercise 1.6. If $g : M \rightarrow M$ is a diffeomorphism of M , then $g \circ \Phi_t \circ g^{-1}$ is the flow of the push-forward field $g_* X$. In particular, if X is invariant under g , so that $g_* X = X$, then the flow of X commutes with g .

Exercise 1.7. Let X, Y be two smooth vector fields on M with respective flows Φ_t^X and Φ_s^Y . Then

$$\frac{d}{dt} \Phi_t^X * Y = -\Phi_t^X [X, Y].$$

Conclude that if X, Y are commuting vector fields, that is, $[X, Y] = 0$, then $\Phi_t^X * Y = Y$ and the flows commute: $\Phi_t^X \circ \Phi_s^Y = \Phi_s^Y \circ \Phi_t^X$.

Exercise 1.8. Let X and Y be vector fields satisfying the Lie bracket relation $[X, Y] = cY$, for a constant c . Show that the flows of X and Y satisfy the relation

$$\Phi_t^X \circ \Phi_s^Y = \Phi_{e^{-ct}s}^Y \circ \Phi_t^X.$$

1.3 MATRIX LIE GROUPS

By a *matrix Lie group* we mean a closed subgroup G of the general linear group $GL(n, \mathbb{R})$. The general linear group in dimension n is an open subset of $M(n, \mathbb{R})$, which is isomorphic as vector space to \mathbb{R}^{n^2} . It turns out that the closed subgroup G is automatically a smooth submanifold of $M(n, \mathbb{R})$ with the restriction of a smooth atlas of its ambient Euclidean space.

Each element $g \in G$ gives rise to two diffeomorphisms of G , L_g and R_g defined by $L_g h = gh$ and $R_g h = hg$. They are called, respective, the *left* and *right translations* by g . A vector field X on G is said to be *left-invariant* if $L_{g*} X = X$ for all $g \in G$. Clearly, the action of G on itself by left (or right) translations is transitive, so a left invariant vector field is completely determined by its value a single element of G . In particular, each left-invariant vector field on G is completely

determined by its value in the tangent space at the identity element, which we denote by $\mathfrak{g} := T_e G$. In other words, there is an isomorphism of vector spaces between \mathfrak{g} and the space of left-invariant vector fields on G given by the correspondence that associates $A \in \mathfrak{g}$ to

$$g \mapsto X_g^A := (dL_g)_e A.$$

Let Φ_t be the flow of the left-invariant vector field X^A . According to Exercise 1.7, Φ_t commutes with left multiplication by any g , and $\Phi_t(g) = g\Phi_t(e)$. It follows that

$$\Phi_{t+s}(e) = \Phi_t(e)\Phi_s(e).$$

We say that $\sigma(t) := \Phi_t(e)$ is a *one-parameter subgroup* of G . Differentiating the identity $\sigma(t+s) = \sigma(t)\sigma(s)$ in s at $s=0$ gives $\sigma'(0) = A$, $\sigma'(t) = \sigma(t)A$, and so $\sigma(t) = \exp(tA)$ where \exp is matrix exponential. Therefore, we conclude that the flow associated to the left-invariant vector field on G associated to the matrix $A \in \mathfrak{g}$ is given by

$$\Phi_t(g) = g \exp(tA).$$

Exercise 1.9. Show that if $X = X^A$ and $Y = X^B$ are the left-invariant vector fields associated to the matrices $A, B \in \mathfrak{g}$ and Φ_t is the flow of X , then

$$\Phi_{t*} Y = e^{-tA} B e^{tA}.$$

Conclude that the value of the Lie bracket at the identity is

$$[X^A, X^B]_e = [A, B]$$

where the right-hand side is the matrix commutator bracket. Therefore, we have an isomorphism of Lie algebras between $\mathfrak{g} := T_e G$ with the matrix commutator and the space of left invariant vector fields on G with the Lie bracket. Therefore, matrix Lie algebras with bracket operation given by matrix commutator exponentiate to matrix Lie subgroups of the general linear group. Conversely, the tangent space at the identity matrix of a closed subgroup of $GL(n, \mathbb{R})$ is a Lie algebra under matrix commutator, which is isomorphic to the Lie algebra of left-invariant vector fields on the matrix group.

Exercise 1.10 (The special linear group). Let $D(A)$ denote the determinant of an n -by- n matrix A . Let X be any element in the tangent space at the identity matrix of $GL(n, \mathbb{R})$. Then $AX = (dL_A)_I X$ is an element of the tangent space at A of $GL(n, \mathbb{R})$. Show that

$$(dD)_A AX = D(A) \text{Tr}(X)$$

where $\text{Tr}(X)$ is the trace of matrix X . Conclude that the *special linear group* $SL(n, \mathbb{R})$, consisting of all the n -by- n real matrices of determinant 1 (which can be shown to be a Lie subgroup of $GL(n, \mathbb{R})$) has Lie algebra

$$\mathfrak{sl}(n, \mathbb{R}) = \{X \in M(n, \mathbb{R}) : \text{Tr}(X) = 0\}.$$

Exercise 1.11 (The orthogonal group). Let $O(n)$ denote the subgroup of $GL(n, \mathbb{R})$ consisting of all orthogonal matrices, that is, matrices A such that $A^\dagger A = I$. Then $O(n)$ is a closed subgroup of $GL(n, \mathbb{R})$, hence a Lie group. Show that its Lie algebra is

$$\mathfrak{o}(n) = \{X \in M(n, \mathbb{R}) : X^\dagger + X = 0\}.$$

The *special orthogonal group* is defined by the intersection

$$SO(n) := O(n) \cap SL(n, \mathbb{R})$$

and its Lie algebra $\mathfrak{so}(n)$ consists of the skew-symmetric matrices (those in $\mathfrak{o}(n)$) of trace 0.

Exercise 1.12 (The symplectic group). *

Exercise 1.13 (Semidirect products and the Euclidean group). *

1.4 VECTOR BUNDLES AND TENSOR FIELDS

In addition to smooth functions and vector fields, other kinds of smooth *tensor fields* will come up later on, such as the metric tensor and volume forms of a Riemannian manifold or the symplectic form of a Hamiltonian system. This abbreviated introduction to general tensor fields should suffice for our needs.

Let V be a k -dimensional vector space over the real numbers and M an n -dimensional manifold. A *vector bundle* E over M with *typical fiber* V is a manifold E of dimension $n + k$ together with

1. a surjective smooth map $\pi : E \rightarrow M$, called the *bundle projection map*,
2. an open cover \mathcal{U} of M , and for each $U \in \mathcal{U}$ a smooth map $\phi : \pi^{-1}U \rightarrow U \times V$ such that

$$(\pi, \phi) : \pi^{-1}U \rightarrow U \times V$$

is a diffeomorphism, and

3. for each $q \in M$ the restriction of ϕ to $E_q : \pi^{-1}(q)$ is a linear isomorphism onto V .

The dimension of V is called the *rank* of the vector bundle E . You should check that the tangent bundle TM of an n -dimensional manifold M is a vector bundle with typical fiber \mathbb{R}^n , hence of rank n . The map (π, ϕ) is called a *local trivialization* of E (or of π) over U . The family of local trivializations defines a *bundle atlas* for E . The *fiber* of E above $x \in M$ is the vector space $E_x := \pi^{-1}(x)$ isomorphic (though not canonically) to V . Two vector bundles are said to be *isomorphic* if there exists a diffeomorphism between them mapping vector space fibers of one bundle to vector space fibers of the other linearly and isomorphically. A product $E = M \times V$ with the projection map on the first factor, or any vector bundle isomorphic to this product bundle, is said to be a *trivial* vector bundle over M .

Exercise 1.14. The unit n -sphere is the submanifold of \mathbb{R}^{n+1} given by

$$S^n = \{(x_1, \dots, x_{n+1}) \in \mathbb{R}^{n+1} : \|x\|^2 := \sum_1^{n+1} x_i^2 = 1\}.$$

Show that TS^n is a nontrivial vector bundle if $n = 2$, but that it is trivial for $n = 3$.

Other examples of vector bundles can be derived from a vector bundle E by the standard vector space constructions. The *cotangent bundle*, T^*M is the vector bundle over M whose fibers are the dual spaces T_x^*M of T_xM for each $x \in M$. More general, we can define the dual vector bundle E^* associated to a given E . If E and F are vector bundles over M , we can define their direct sum $E \oplus F$, which is a vector bundle of M whose fibers are the direct sums of the corresponding fibers of E and F . Similarly, one may define the tensor product $E \otimes F$, and more general tensor bundles, such as $E^* \otimes E \otimes F$, etc. The tensor bundle over M of *type* (r, s) derived from a vector bundle E is

$$T_s^r(E) = \underbrace{E \otimes \cdots \otimes E}_r \otimes \underbrace{E^* \otimes \cdots \otimes E^*}_s.$$

Typically, we will be interested in $E = TM$ and various associated tensor bundles, such as T^*M , $TM \otimes T^*M$, and subbundles of $T^*M \otimes T^*M$.

A *section* of a vector bundle E over M is a map $\sigma : M \rightarrow E$ such that $\sigma(x)$ belongs to E_x for all $x \in M$. For example, a vector field is a section of the tangent bundle TM . A covector field is a section of the cotangent bundle T^*M . *Tensor fields* over M are sections of tensor bundles derived from TM . A tensor field of type (r, s) is a section of $T_s^r(TM)$. Concrete examples of these concepts will appear over the course of these lectures.

If (x_1, \dots, x_m) is a coordinate system on an open set U in an m -dimensional manifold M , then the partial derivative $\frac{\partial}{\partial x_j}$ constitute a basis of the tangent spaces at each point in U . The dual coordinate basis for T_x^*M at each $x \in U$ is $\{dx_1, \dots, dx_m\}$. By definition, the dual basis is characterized by the values of the pairings of basis elements: $dx_i(\frac{\partial}{\partial x_j}) = \delta_{ij}$, where δ_{ij} is 1 when $i = j$ and 0 otherwise. A coordinate basis of the tensor spaces $T_s^r(TM)$ at each x in U is obtained by taking tensor products. The typical element of the basis has the form

$$\partial_{x_{i_1}} \otimes \cdots \otimes \partial_{x_{i_r}} \otimes dx_{j_1} \otimes \cdots \otimes dx_{j_s}.$$

1.5 DIFFERENTIAL FORMS

We summarize here the main facts concerning differential forms and integration of forms on manifolds. All functions and maps will by default be assumed smooth.

Definition 1.2. A differential 1-form ω over an open set U in \mathbb{R}^n is a map from U taking values in the dual space of \mathbb{R}^n . In the standard coordinates of \mathbb{R}^n , a differential 1-form is written as

$$\omega = \sum_{j=1}^n f_j(x) dx_j.$$

If f is a function on \mathbb{R}^n , the *differential* of f is the 1-form defined by $df = \sum_{j=1}^n \frac{\partial f}{\partial x_j}(x) dx_j$. If $\gamma = (\gamma_1, \dots, \gamma_n) : [a, b] \rightarrow U$ is a smooth path in U , the integral of ω along γ is defined by

$$\int_{\gamma} \omega := \int_a^b \sum_{j=1}^n f_j(\gamma(t)) \gamma_j'(t) dt.$$

In particular, $\int_{\gamma} df = f(\gamma(b)) - f(\gamma(a))$.

Definition 1.3. An alternating k -form on a vector space V is a map $\Phi : \underbrace{V \times \cdots \times V}_k \rightarrow \mathbb{R}$ that is linear in each vector argument and is antisymmetric:

$$\Phi(u_{\sigma(1)}, \dots, u_{\sigma(k)}) = \epsilon(\sigma) \Phi(u_1, \dots, u_k)$$

where σ is an element of the permutation group S_k on the indices $\{1, \dots, k\}$ and $\epsilon(\sigma)$ denotes the sign of the permutation (+ for an even and - for an odd permutation). The space of all alternating k -forms on V is naturally a vector space, denoted $\Lambda^k(V)$.

Definition 1.4. A differential k -form on the open subset U of \mathbb{R}^n is a smooth function from U into the space $\Lambda^k(\mathbb{R}^n)$ of alternating k -forms in \mathbb{R}^n .

If $\varphi_1, \dots, \varphi_k$ are elements in the dual space of \mathbb{R}^n , then

$$\Phi(u_1, \dots, u_k) := \sum_{\sigma \in S_k} \epsilon(\sigma) \varphi_1(u_{\sigma(1)}) \cdots \varphi_k(u_{\sigma(k)})$$

is easily seen to be an alternating k -form.

Definition 1.5. We define the differential k -form $dx_{i_1} \wedge \cdots \wedge dx_{i_k}$ on \mathbb{R}^n by

$$dx_{i_1} \wedge \cdots \wedge dx_{i_k}(u_1, \dots, u_k) := \sum_{\sigma \in S_k} \epsilon(\sigma) dx_{i_1}(u_{\sigma(1)}) \cdots dx_{i_k}(u_{\sigma(k)}).$$

It is not difficult to show that every differential k -form ω on an open set U in \mathbb{R}^n can be written at each x as

$$\omega_x = \sum_{1 \leq i_1 < \cdots < i_k \leq n} f_{i_1 \dots i_k}(x) dx_{i_1} \wedge \cdots \wedge dx_{i_k}$$

where the $f_{i_1 \dots i_k}$ are smooth real-valued functions on U .

Definition 1.6. The space of all smooth k -forms on U will be denoted $\Omega^k(U)$. The set of all smooth forms on U is the vector space given by the direct sum

$$\Omega(U) = \Omega^0(U) \oplus \cdots \oplus \Omega^n(U),$$

where $\Omega^0(U)$ is the space of smooth functions on U . If α is a differential k -form on U and β is a differential l -form on U , the *wedge product* $\alpha \wedge \beta$ is the differential $(k+l)$ -form on U defined by

$$(\alpha \wedge \beta)_x(u_1, \dots, u_{k+l}) = \frac{1}{k!l!} \sum_{\sigma \in S_{k+l}} \epsilon(\sigma) \alpha_x(u_{\sigma(1)}, \dots, u_{\sigma(k)}) \beta_x(u_{\sigma(k+1)}, \dots, u_{\sigma(k+l)}).$$

The wedge product \wedge makes $\Omega(U)$ a graded algebra called the *exterior algebra*.

We have already defined the differential $d : \Omega^0(U) \rightarrow \Omega^1(U)$ by $df = \sum \frac{\partial f}{\partial x_j} dx_j$. It is not difficult to show that this d can be extended uniquely to all of $\Omega(U)$ in such a way that the following properties hold:

1. $d : \Omega^k(U) \rightarrow \Omega^{k+1}(U)$
2. d is a linear operation
3. $d(df) = 0$
4. $d(\alpha \wedge \beta) = d\alpha \wedge \beta + (-1)^k \alpha \wedge d\beta$, where $\alpha \in \Omega^k(U)$.

We call $d\alpha$ the *exterior derivative* of α . If $d\alpha = 0$ we say that α is a *closed* form, and if $\alpha = d\eta$ for some differential form η we say that α is an *exact* form.

Definition 1.7. Let $\varphi : U \rightarrow V$ be a smooth diffeomorphism between two open sets in \mathbb{R}^n and let $\omega \in \Omega^k(V)$. The *pull-back* of ω under φ is the differential k -form $\varphi^* \omega$ in $\Omega^k(U)$ defined by

$$(\varphi^* \omega)_x(u_1, \dots, u_k) = \omega_{\varphi(x)}(d\varphi_x u_1, \dots, d\varphi_x u_k).$$

Note that $d\varphi$ is the general differential of a map defined earlier.

We use d for essentially two different concepts of differentiation. When φ is a map between two manifolds, $d\varphi_x$ is the linear (Jacobian) map induced on tangent spaces, whereas $d\omega$, when ω is a differential form, is the exterior derivative. There is little risk of confusion in this. Only when φ is a function (that is, a map into \mathbb{R}) could there be any ambiguity in deciding between the two meanings of df , and in this case the two meanings are directly related. In fact, as a one form, $df(u) = uf$, the derivative of f in the direction of u , and as the differential of the map f , $df(u) = uf \frac{d}{dx}$, where $\frac{d}{dx}$ is the coordinate vector field on \mathbb{R} . Under the identification of tangent vectors in \mathbb{R} with their numerical component $a \frac{d}{dx} \leftrightarrow a$ the two meanings of df coincide.

It is now not difficult to show that the concepts of differential forms, the wedge product, the exterior derivative, and the pull-back of forms naturally extend from open sets of \mathbb{R}^n to general manifolds. If $\omega \in \Omega^k(M)$ then ω_q is an alternating k -form on $T_q M$ for each $q \in M$. It can also be shown that if $\varphi : M \rightarrow N$ is a smooth map and α, β are differential forms on N , then

1. $\varphi^*(\alpha \wedge \beta) = \varphi^* \alpha \wedge \varphi^* \beta$
2. $\varphi^* d\alpha = d\varphi^* \alpha$
3. $dd = 0$
4. $d(\alpha \wedge \beta) = d\alpha \wedge \beta + (-1)^k \alpha \wedge d\beta$, where $\alpha \in \Omega^k(N)$.

We now consider the properties relating differential forms, vector fields, and flows. A useful operation involving vector fields and differential forms is the *interior product*, defined as follows.

Definition 1.8. Let X be a smooth vector field and ω a differential k -form on M . Then $i_X \omega$, also denoted $X \lrcorner \omega$, is the $(k-1)$ -form defined by

$$(i_X \omega)_q(u_1, \dots, u_{k-1}) = \omega(X_q, u_1, \dots, u_{k-1}).$$

When ω is a 0-form we define $i_X \omega = 0$.

The following properties characterize the operation i_X on differential forms.

1. $i_X f = Xf$ where f is a smooth function.
2. $i_X(\alpha \wedge \beta) = (i_X \alpha) \wedge \beta + (-1)^k \alpha \wedge (i_X \beta)$ where α is a k -form.

Definition 1.9. Let X be a smooth vector field on a manifold M with associated (local) flow Φ_t and let ω be a differential form. The Lie derivative of ω along X is defined to be

$$L_X \omega := \left. \frac{d}{dt} \right|_{t=0} \Phi_t^* \omega.$$

The Lie derivative of forms has the following properties.

1. $L_X f = Xf$ if $f \in \Omega^0(M)$
2. $L_X d\omega = dL_X \omega$
3. $L_X(\alpha \wedge \beta) = (L_X \alpha) \wedge \beta + \alpha \wedge (L_X \beta)$
4. $L_X \omega = di_X \omega + i_X d\omega$
5. $\frac{d}{dt}(\Phi_t^* \omega) = \Phi_t^*(L_X \omega)$.

The *support* of a differential form on M is the closure of the set $\{q \in M : \omega_q \neq 0\}$. Let $\omega = f dx_1 \wedge \dots \wedge dx_n$ be an n -form on \mathbb{R}^n with compact support contained in an open set $U \subset \mathbb{R}^n$. The integral of ω over U is defined to be

$$\int_U \omega = \int_U f(x_1, \dots, x_n) dx_1 \dots dx_n$$

where $dx = dx_1 \dots dx_n$ is the Lebesgue measure on \mathbb{R}^n .

If $\varphi : U \rightarrow V$ is a diffeomorphism between two open sets in \mathbb{R}^n , we say that φ preserves orientation if $\varphi^*(dx_1 \wedge \dots \wedge dx_n)_x = f(x) dx_1 \wedge \dots \wedge dx_n$, where $f(x) > 0$ for all $x \in U$. Two overlapping coordinate charts on an n -dimensional manifold M are said to have the same orientation if the associated change of coordinates diffeomorphism between open sets in \mathbb{R}^n is orientation preserving. The manifold M is said to be *orientable* if it is possible to find a subatlas of the atlas describing M as a smooth manifold consisting of compatibly oriented coordinate charts. A choice of orientation on M is a choice of such a sub-atlas.

Theorem 1.1. Let M be an n -dimensional orientable manifold. There exists a real-valued linear functional from the space $\Omega_c^n(M)$ of compactly supported n -forms on M , denoted

$$\omega \mapsto \int_M \omega$$

such that if φ is a diffeomorphism compatible with the orientation from an open set $U \subset \mathbb{R}^n$ onto an open set $V \subset M$ containing the support of ω , then

$$\int_M \omega = \int_U \varphi^* \omega.$$

We denote by \mathbb{H}^n the half-space in \mathbb{R}^n defined by $\mathbb{H}^n := \{x \in \mathbb{R}^n : x_n \geq 0\}$.

Definition 1.10 (Manifold with boundary and boundary orientation). *

Theorem 1.2 (Stokes theorem). Let M be an orientable manifold of dimension n and let $j : \partial M \rightarrow M$ be the canonical inclusion of the boundary of M into M . We assume that ∂M has the induced boundary orientation. Then for any compactly supported $(n-1)$ -form ω one has

$$\int_M d\omega = \int_{\partial M} j^* \omega.$$

2 NEWTONIAN MECHANICAL SYSTEMS

2.1 CONFIGURATION MANIFOLDS AND THE KINETIC ENERGY METRIC

We now turn to classical (Newtonian) mechanical systems. It may be appropriate to begin by stating a general definition of what we are going to understand by a *mechanical system* and, more specifically, a *billiard-like system* (or a system of *billiard type*). This section will contain more differential geometry than strictly necessary for the rest of the lectures, but it may, we hope, provide some helpful perspective into the variety of examples of systems we are going to encounter. Briefly, we use the term *Newtonian mechanical system* to refer to non-relativistic, classical (as opposed to quantum) systems whose Lagrangian function (to be introduced shortly) has the form of a kinetic energy function minus a potential function. In particular, we do not consider dissipative forces such as friction or viscosity. Some understanding of dissipative phenomena will be gained nevertheless when we look into statistical mechanics later on. For most of the systems we are going to explore, which will be of the billiard type, even potential forces will be absent and the only type of interaction between the material parts of the system will be through elastic collisions.

Definition 2.1 (System of masses and manifold of configurations). The following data define a system of masses comprising the mechanical system and the space of possible configurations these masses can assume in coordinate space \mathbb{R}^n . Typically, $n \leq 3$.

1. \mathcal{B} denotes a Borel measurable space with a finite (positive) measure μ that specifies the mass distribution. The *total mass* is $m = \mu(\mathcal{B})$, hence a fixed subset of \mathbb{R}^n . We think of \mathcal{B} as the *material body* in some fixed, or reference, configuration.
2. The *configuration manifold* M is a smooth manifold with *corners* as defined in [5]. (The boundary may be empty.) The dimension of M specifies the *degrees of freedom* of motions of the body.
3. The *position map* $\Phi : M \times \mathcal{B} \rightarrow \mathbb{R}^n$ assigns for each *material point* $b \in \mathcal{B}$ and $q \in M$ the position $\Phi(q, b)$ of b in the configuration q . We assume that $q \mapsto \Phi(q, b)$ is a smooth map for each b . Any of the equivalent notations $\Phi(q, b) = \Phi_q(b) = \Phi_b(q) = q(b)$ may be used.

The following simple example (see Figure 1) should help to clarify Definition 2.1. It consists of a pendulum with a circular bob of radius r rigidly attached to the end of a rod so that the

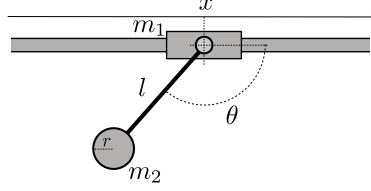


Figure 1: A disc of mass m is attached to the end of a rigid rod that swings freely about a pivot point. The pivot is mounted on a rail, along which it can slide without friction. The distance from the pivot to the center of the disc is l . The configuration manifold is topologically a cylinder parametrized by $(x, [\theta]) \in \mathbb{R} \times \mathbb{T}$, where \mathbb{T} denotes the interval $[0, 2\pi]$ with the endpoints 0 and 2π identified.

distance from the pivot to the center of the bob is l . The pendulum pivot rotates freely (without friction) and slides freely along a horizontal rail. The sliding part of the system to which the pivot is attached has mass m_1 , assumed (with no loss of generality) to be concentrated at the pivot point. The rest of the mass of the system, m_2 , is distributed uniformly over the pendulum bob. We let $\mathcal{B}_1 = \{0\}$ (the origin of \mathbb{R}^2) represent the pivot and $\mathcal{B}_2 = \{(b_1, b_2) \in \mathbb{R}^2 : b_1^2 + b_2^2 \leq r^2\}$ the bob, and write $\mathcal{B} = \mathcal{B}_1 \cup \mathcal{B}_2$, where the union should be understood to be disjoint. (Note that the various components of \mathcal{B} are allowed to overlap. Strictly speaking, one should add an index to these components in order to be clear that one is dealing with a disjoint union, something we will not do for the sake of keeping the notation simple. Typically, $\Phi(q, \cdot)$ will separate these overlapping components.) The mass distribution is then $d\mu(b) = (m_2/\pi r^2) db_1 db_2$ for $b \in \mathcal{B}_2$ and $\mu(0) = m_1$ if $0 \in \mathcal{B}_1$. The manifold of configurations is $M = \mathbb{R} \times \mathbb{T}$, where $\mathbb{T} = \mathbb{R}/2\pi\mathbb{Z}$. Equivalently, we may view \mathbb{T} as the unit circle, so M is diffeomorphic to a cylinder. A point $q = (x, [\theta])$ represents a configuration in which the pendulum pivot is at position x along the rail and the pendulum arm is at an angle θ relative to the line of the rail. Here $[\theta]$ represents the equivalence class module 2π .

We may describe the position map for this example as follows. Let $e_1 = (1, 0)^\dagger$, $e_2 = (0, 1)^\dagger$ be the standard basis vectors in \mathbb{R}^2 , regarded as column vectors. (The superscript ‘ \dagger ’ indicates matrix transpose.) Let R_θ denote the 2-by-2 matrix representing rotation counterclockwise by angle θ and $b = (b_1, b_2)^\dagger$. Then

$$(2.1) \quad \Phi((x, [\theta]), b) = \begin{cases} x & \text{if } b \in \mathcal{B}_1 \\ R_\theta(b + le_1) + xe_1 & \text{if } b \in \mathcal{B}_2 \end{cases}$$

2.2 THE EULER-LAGRANGE EQUATIONS

Definition 2.2 (Motions and states). Given a mechanical system (\mathcal{B}, μ, Φ) with configuration manifold M , we define a *motion* of the system to be a path $\gamma : I \rightarrow M$ where I is some interval in \mathbb{R} . A (pure) *state* of the system is an element of the tangent bundle TM . We denote a state by the pair (q, v) , where $q \in M$ and $v \in T_q M$. (Later on, a state will be understood more generally as a probability measure on M . If the measure is supported on a single point we say that it is a

pure state.)

Given a state $\xi = (q, v)$, we introduce a vector field on $\mathcal{B} \subset \mathbb{R}^n$ as follows. Let $\gamma : (-a, a) \rightarrow M$ be a path *representing* (q, v) . That is, a differentiable path such that $\gamma(0) = q$ and $\gamma'(0) = v$. Then the vector field, which we also denote by ξ , is

$$\xi(b) := \left. \frac{d}{dt} \right|_{t=0} \Phi(\gamma(t), b).$$

We think of the path parameter t as ‘time’ and call $b \mapsto \xi(b)$ the *velocity field* on \mathcal{B} corresponding to the state $\xi \in TM$. If $\gamma(t)$ is given in terms of coordinates (q_1, \dots, q_n) on M , we typically denote time derivative of the coordinate functions by \dot{q}_j .

Definition 2.3 (Kinetic energy metric). Given (\mathcal{B}, μ, Φ) with configuration manifold M , we define on TM a field of symmetric bilinear forms $q \mapsto \langle \cdot, \cdot \rangle_q$ as follows. For any two states $\xi = (q, u), \eta = (q, v)$ at $q \in M$ we define

$$\langle u, v \rangle_q := \int_{\mathcal{B}} \xi(q) \cdot \eta(b) d\mu(b)$$

where $\xi(q) \cdot \eta(b)$ indicates the standard inner product (dot-product) in \mathbb{R}^n . We always make the (very weak) assumption that the position map is *effective* in that $\langle \cdot, \cdot \rangle_q$ is a non-degenerate symmetric form at each q . In other words, it defines a Riemannian metric on M . The *kinetic energy* function is by definition the function $K : TM \rightarrow [0, \infty)$ given by

$$K(q, v) = \frac{1}{2} \|v\|_q^2.$$

Notice how the mass distribution given by the measure μ is incorporated into the norm $\|\cdot\|$.

As an example let us calculate the kinetic energy function for the system of Figure 1. The rotation matrix is $R_\theta = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$ and its time derivative for a motion described in coordinates by $(x(t), [\theta(t)])$ is the matrix $\dot{\theta} R_{\theta + \frac{\pi}{2}}$. Therefore, taking the derivative in t (at $t = 0$) of $\Phi((x(t), [\theta(t)]), b)$ (see Equation 2.1) gives

$$\xi(b) = \begin{cases} \dot{x} e_1 & \text{if } b = 0 \in \mathcal{B}_1 \\ \dot{\theta} R_{\theta + \frac{\pi}{2}}(b + l e_1) + \dot{x} e_1 & \text{if } b \in \mathcal{B}_2 \end{cases}$$

A simple calculation now gives the kinetic energy function evaluated at a tangent vector $v = (\dot{x}, \dot{\theta})$ of M , expressed in the coordinates $q = (x, \theta)$, as

$$K(q, v) = \frac{1}{2} \int_{\mathcal{B}} |\xi(b)|^2 d\mu(b) = \frac{1}{2} m_1 \dot{x}^2 + \frac{1}{2} m_2 \left[\left(\frac{r^2}{2} + l^2 \right) \dot{\theta}^2 + \dot{x}^2 - 2\dot{x}\dot{\theta}l \sin \theta \right].$$

The dynamics of the mechanical system is introduced through a choice of *Lagrangian* function on the phase space TM .

Definition 2.4 (Lagrangian and action functional). The Lagrangian of a Newtonian mechanical system is the function $L: TM \rightarrow \mathbb{R}$ defined on the tangent bundle (the *phase space* of the system) TM and given by

$$L(q, v) := K(q, v) - V(q)$$

where $V(q)$ is a *potential energy* function on M . If $\gamma: [a, b] \rightarrow M$ is a differentiable path describing a motion of the system, the *action functional* evaluated on γ is

$$S[\gamma] := \int_a^b L(\gamma(t), \gamma'(t)) dt.$$

According to Hamilton's principle of stationary action, a path $\gamma(t)$ describing an actual physical motion of the system must be a critical path of the action functional. To state the principle in more detail we first define a *variation* of a path $\gamma(t)$ with fixed endpoints.

Definition 2.5 (Variation of a critical path). Let $\gamma: [a, b] \rightarrow M$ be a smooth path. A smooth *variation* of γ with endpoints fixed is a smooth map $\Gamma: [a, b] \times (-\epsilon, \epsilon) \rightarrow M$, for some $\epsilon > 0$, such that for all $t \in [a, b]$ and $s \in (-\epsilon, \epsilon)$,

$$\Gamma(t, 0) = \gamma(t), \quad \Gamma(a, s) = \gamma(a), \quad \Gamma(b, s) = \gamma(b).$$

We denote by Γ_s and Γ_t the partial derivatives of Γ in the first and second variables, respectively. Given a Lagrangian function $L: TM \rightarrow \mathbb{R}$ and its associated action functional S , γ is a *critical path* for S if for any smooth variation Γ of γ

$$\left. \frac{d}{ds} \right|_{s=0} S[\Gamma(\cdot, s)] := \left. \frac{d}{ds} \right|_{s=0} \int_a^b L(\Gamma(t, s), \Gamma_t(t, s)) dt = 0.$$

We call a critical path of the action functional an *L-critical path*.

Hamilton's principle of stationary action: For a path $t \mapsto \gamma(t)$ in M to represent an actual physical motion of the mechanical system (\mathcal{B}, μ, Φ) with Lagrangian L , γ must be *L-critical*.

Theorem 2.1 (The Euler-Lagrange equations in local coordinates). Let the *L-critical* path γ lie in a coordinate chart with domain U in the configuration manifold M . Let (q_1, \dots, q_n) be the coordinate functions on U and $(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n)$ be the induced coordinate function on $TU \subset TM$, consisting of tangent vectors having base point in U . In these coordinates the Lagrangian has the form $L(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n)$. Then γ must satisfy the n equations:

$$\frac{\partial L}{\partial q_j}(\gamma(t), \gamma'(t)) - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j}(\gamma(t), \gamma'(t)) \right) = 0.$$

Proof. Let $\gamma(t)$ be an *L-critical* path and $\Gamma(t, s)$ a variation of γ . We write, with slight (but conventional) abuse of notation

$$L(\Gamma(t, s), \Gamma_t(t, s)) = L(q_1(t, s), \dots, \dot{q}_n(t, s))$$

and observe that

$$\frac{\partial}{\partial s} L(q_1(t, s), \dots, \dot{q}_n(t, s)) = \sum_{j=1}^n \left(\frac{\partial L}{\partial q_j} - \frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{q}_j} \right) \right) \frac{\partial q_j}{\partial s} + \frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{q}_j} \frac{\partial q_j}{\partial s} \right).$$

Setting $V_j(t) = \frac{\partial q_j}{\partial s}(t, 0)$ and noting that $V_j(a) = V_j(b) = 0$, we obtain

$$0 = \frac{d}{ds} \Big|_{s=0} \int_a^b L(\Gamma(t, s), \Gamma_t(t, s)) dt = \int_a^b \sum_{j=1}^n \left(\frac{\partial L}{\partial q_j} - \frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{q}_j} \right) \right) V_j(t) dt.$$

The variation vector field $(V_1(t), \dots, V_n(t))$ can be chosen arbitrarily except for the condition that it vanishes at $t = a, b$. It follows that $\frac{\partial L}{\partial q_j} - \frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{q}_j} \right) = 0$ for each j and all $t \in [a, b]$. \square

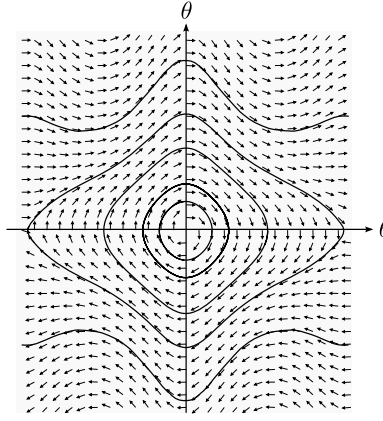


Figure 2: Expressing the second order equation in θ given in part 3 of this exercise as a system of two first order equations in the $(\theta, \dot{\theta})$ -plane produces this direction field.

Consider again the example of Figure 1. Let us suppose that the system is subject to gravitational potential of the form

$$V(q) = g \int_{\mathcal{B}} \Phi(q, b) \cdot e_2 d\mu(b)$$

where g is acceleration due to gravity. This expression should be interpreted as follows. At a configuration $q \in M$ the height (relative to some arbitrarily chosen ground level) of the material point b is $\Phi(q, b) \cdot e_2$ and the amount of mass at this height around b is $d\mu(b)$. The contribution to the gravitational potential energy (near the surface of the Earth) of a particle of matter is its height times its mass times the constant g . The integral over \mathcal{B} then gives the total potential energy of the body. An integral calculation using the expression 2.1 yields the physically obvious result: $V(x, [\theta]) = gm_2 l \sin \theta$. (Note that θ , for the configuration shown in Figure 1, is negative and that we omit the contribution of m_1 to the potential function since the pendulum pivot remains at a constant height.) The Lagrangian function for the pendulum-on-a rail system is then

$$L(x, [\theta], \dot{x}, \dot{\theta}) = \frac{1}{2} (m_1 + m_2) \dot{x}^2 + \frac{1}{2} m_2 \left[\left(\frac{r^2}{2} + l^2 \right) \dot{\theta}^2 - 2\dot{x}\dot{\theta} l \sin \theta \right] - gm_2 l \sin \theta.$$

Note the term $m_2 r^2 \dot{\theta}^2 / 4$ in the kinetic energy. It represents the rotational energy of the bob, which rotates with the same angular speed as the rod itself.

It is now easy to obtain the equations of motion, which are the two equations (in x and θ) obtained from Theorem 2.1. They are described in the next exercise.

Exercise 2.1 (Pendulum on a rail). Derive the following facts for the system of Figure 1.

1. The Euler-Lagrange equations are

$$\begin{aligned} \bullet \quad 0 &= \frac{\partial L}{\partial x} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) = -(m_1 + m_2) \ddot{x} + m_2 l \ddot{\theta} \sin \theta + m_2 l \dot{\theta}^2 \cos \theta \\ \bullet \quad 0 &= \frac{\partial L}{\partial \theta} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\theta}} \right) = \frac{1}{2} m_2 \left[(r^2 + 2l^2) \ddot{\theta} - 2\ddot{x} l \sin \theta \right] + g m_2 l \cos \theta. \end{aligned}$$

2. Define $x_c = x + \frac{m_2}{m_1 + m_2} l \cos \theta$, the horizontal component of the *center of mass* of the system. Using the first of the Euler-Lagrange equations show that $\ddot{x}_c = 0$. Therefore, $x_c = v_c t + x_c(0)$, where v_c is the constant velocity of x_c . Therefore,

$$x(t) = a + bt - \frac{m_2}{m_1 + m_2} l \cos \theta(t)$$

where the constants a, b are specified by a choice of initial conditions.

3. Show that θ satisfies the differential equation

$$\left[\frac{1}{2} (r^2 + 2l^2) - \frac{m_2}{m_1 + m_2} l^2 \sin^2 \theta \right] \ddot{\theta} - \frac{m_2}{m_1 + m_2} l^2 (\sin \theta \cos \theta) \dot{\theta}^2 + g l \cos \theta = 0.$$

4. Express the equation of part 3 as a system of first order equations in θ and $\dot{\theta}$. This system can be interpreted as the vector field on the plane \mathbb{R}^2 . The corresponding field of directions (not taking into account the magnitude of the vectors) is shown in Figure 2. A few integral curves are also shown.
5. When $m_1 = \infty$ and $r = 0$, the previous equation reduces to the standard equation of motion of the simple pendulum:

$$\ddot{\theta} + \frac{g}{l} \cos \theta = 0.$$

6. If $r = 0$ and $m_1 = 0$, show that the differential equation for θ obtained in part 3 reduces to

$$\left(\ddot{y} + \frac{g}{l} \right) \cos \theta = 0$$

where $y = \sin \theta$. Does this equation make physical sense? (If $\cos \theta \neq 0$, $\ddot{y} + g/l = 0$ implies that the bob is in free-fall. When $\cos \theta = 0$ the rigidity of rod suddenly manifests itself.)

Exercise 2.2 (Double pendulum on a rail). Obtain the position map and Lagrangian for the double pendulum shown in Figure 3. The symbol 0 indicates the origin of \mathbb{R}^2 . The position map restricted to $\mathcal{B}_1 \cup \mathcal{B}_2$ is just like the position map of Exercise 2.1. The body now consists of three component parts: $\mathcal{B} = \mathcal{B}_0 \cup \mathcal{B}_1 \cup \mathcal{B}_2$, where $\mathcal{B}_0 = \{0\}$ is the origin of \mathbb{R}^2 and represents

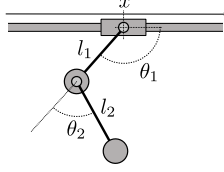


Figure 3: A double pendulum. Now the configuration manifold is $\mathbb{R} \times \mathbb{T}^2$ where $\mathbb{T}^2 = \mathbb{R}^2 / (2\pi\mathbb{Z})^2$.

the sliding part on the rail containing the pivot, and \mathcal{B}_i is the disc of radius r_i centered at the origin, for $i = 1, 2$. (As before, the union of the parts should be understood in the sense of disjoint union.) Give the parts uniform mass distribution with total masses m_0, m_1, m_2 . In order to obtain the position map restricted to the second bob, we suggest using the sequence of transformations indicated in Figure 4

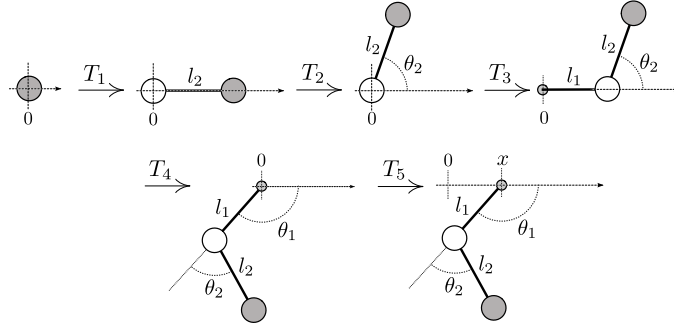


Figure 4: The position map restricted to \mathcal{B}_2 may be described using the composition of maps $\Phi(q, b) = (T_5 \circ \dots \circ T_1)(b)$ as indicated in the figure, where $q = (x, [\theta_1], [\theta_2])$ and the T_j are either translations in the direction e_1 or rotations. More specifically, define $\tau_x(b) = b + xe_1$. Then $T_1(b) = \tau_{l_2}$, $T_2 = R_{\theta_2}$, $T_3 = \tau_{l_1}$, $T_4 = R_{\theta_1}$ and $T_5 = \tau_x$.

Exercise 2.3. Consider the system shown in Figure 5. A point mass m slides freely on a circular rail of radius r . The rail rotates about the vertical axis through its center at constant angular velocity ω and acceleration due to gravity is assumed to be constant, equal to g . Let the configuration manifold M be \mathbb{T} parametrized by the angle θ , $\mathcal{B} = \{0\}$, and $\Phi([\theta], 0) = (x, y, z)$ where

$$x = r \sin \theta \cos(\omega t), \quad y = r \sin \theta \sin(\omega t), \quad z = r \cos \theta.$$

1. Write down the position map, the Lagrangian function and the equations of motion (the Euler-Lagrange equations) for this system.

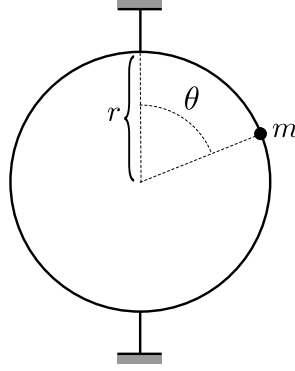


Figure 5: Illustration for Exercise 2.3. A point mass m slides freely on a circular rail that rotates at constant angular speed about the vertical axis. The configuration manifold is \mathbb{T} . Assume constant acceleration due to gravity g .

2. Show that the Euler-Lagrange equation can be written in the form

$$\ddot{\theta} = \omega^2 \sin \theta \cos \theta + \frac{g}{r} \sin \theta.$$

3. Let $x_1 = \theta$, $x_2 = \dot{\theta}$. Show that the second order equation in θ corresponds to the system

- $\dot{x}_1 = x_2$
- $\dot{x}_2 = \frac{g}{r} (\alpha \cos x_1 - 1) \sin x_1$

where $\alpha = r\omega^2/g$.

4. Show that the critical points of the system (points where $\dot{x}_1 = \dot{x}_2 = 0$) are given by $(x_1, 0)$ where $x_1 = 0, \pm\pi$, and $\arccos(1/\alpha)$ when $\alpha \geq 1$.
5. Describe the physical behavior of the system near each critical point and draw a phase portrait similar to Figure 2.

2.3 VIBRATING SYSTEMS

Exercise 2.4 (Spring-mass systems-I). In this and the next few exercises we explore vibrating system near equilibrium configurations. Let the configuration manifold be \mathbb{R} . The variable $x \in \mathbb{R}$ represents the position of the block of mass m as indicated in Figure 6. The potential function of this system (assuming ideal linear spring) is taken to be $U(x) = \frac{1}{2} kx^2$, where k is called the *spring constant*, and the the Lagrangian function is $L(x, \dot{x}) = \frac{1}{2} m\dot{x}^2 - \frac{1}{2} kx^2$. Show that the general solution to the Euler-Lagrange equation is

$$x(t) = A \cos\left(\sqrt{\frac{k}{m}} t\right) + B \sin\left(\sqrt{\frac{k}{m}} t\right)$$

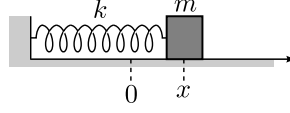


Figure 6: The simplest spring-mass system. The point marked 0 indicates the position of the freely sliding block of mass m when the spring is neither compressed nor stretched.

where A and B are constants obtained from the initial position and velocity of the (center of the) block. $T = 2\pi\sqrt{m/k}$ is called the *period of oscillation*. It is the physical dimension of time.

Exercise 2.5 (Spring-mass systems-II). This exercise is a preliminary step towards dealing with a class of networks of springs. The spring-mass system depicted in Figure 7 consists of two masses that can slide freely along poles. We consider no forces other than the potential force between the masses due to a spring of constant k . The position (height) of each mass in its pole is denoted $\phi(i)$. The potential function for this system is $U(\phi_1, \phi_2) = \frac{1}{2}k(\bar{L} - l)^2$ where $\bar{L}^2 = L^2 + (\phi_1 - \phi_2)^2$.

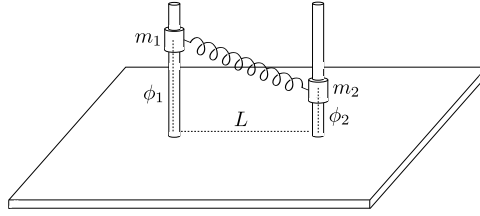


Figure 7: System of Exercise 2.5. The distance between the base points of the two poles is L , the length of the relaxed string is $l < L$ and the actual length of the spring is \bar{L} .

Show that $\frac{\partial U}{\partial \phi_1} = \beta_{21}(\phi_1 - \phi_2)$ where, for small values of $\delta := ((\phi_1 - \phi_2)/L)^2$,

$$\beta_{21} = k \left(1 - \frac{l}{L} \right) + O(k\delta).$$

This justifies dropping terms of order 1 or greater in δ and approximating β by a constant.

The system of springs and masses considered in the next exercise has the following general description. We think of \mathbb{R}^2 as flat horizontal board to each are attached long pins (or poles) at positions $\mathcal{P} = \{x_1, \dots, x_k\} \subset \mathbb{R}^2$. We distinguish two types of pins: The *interior* set $\mathcal{P}_0 \subset \mathcal{P}$, which contain the sliding point masses, and the set of *boundary* pins $\partial\mathcal{P} = \mathcal{P} \setminus \mathcal{P}_0$. The boundary pins are those to which spring-ends are attached at fixed heights. A configuration of the system of masses is a function $\phi : \mathcal{P} \rightarrow \mathbb{R}$. For simplicity we assume that a point mass can have any height value; that is, we ignore the lower bound on ϕ suggested by the image of a “floor” \mathbb{R}^2 in our description of the system. The height of a point mass above $x_j \in \mathcal{P}_0$ at a given time t will be written $\phi(x_j, t) = \phi_j(t)$. Heights at points in the boundary set $\partial\mathcal{P}$ are fixed and given by some

function f . So we write the boundary condition by the expression $\phi|_{\partial\mathcal{P}} = f$. In the example of Figure 8 (a view from above of the system) the boundary set is indicated by the white circle vertices and the interior points containing the sliding masses are the shaded discs.

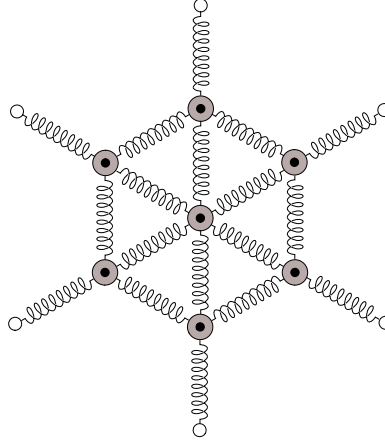


Figure 8: A system of sliding masses and springs viewed from the top. The masses are represented by the shaded discs with black centers. The white circles are end points of springs that are kept at a fixed height. Either kind has a fixed base point in \mathbb{R}^2 , so the configuration of the system is fully specified by the heights $\phi(j)$. (This means that the motion of the system is not apparent when looked at from above as in this figure.)

We now define the spring-mass mechanical system formally by the following data. The configuration manifold is $M = \{\phi : \mathcal{P} \rightarrow \mathbb{R} \text{ such that } \phi|_{\partial\mathcal{P}} = f\}$. The body may be identified with the indices of the interior pins. If the number of these is $l < k$, a convenient choice of indices is $\mathcal{B} = \{1, \dots, l\}$. The mass distribution is the measure on \mathcal{B} indicated by $\mu(j) = m_j$. The position map is now

$$\Phi : (\phi, j) \in M \times \mathcal{B} \mapsto (x_j, \phi_j) \in \mathbb{R}^3.$$

We write $\dot{\phi}_j$ for the time derivative of the ϕ_j . Based on the conclusion of Exercise 2.5 we assume the quadratic approximation of the potential function, which now involves all pairs of pins:

$$U(\phi) = \sum_{i < j} \frac{1}{2} \beta_{ij} (\phi_i - \phi_j)^2.$$

We implicitly assume that the spring constant k_{ij} that enters into β_{ij} as described in Exercise 2.5 is 0 if masses m_i and m_j are not connected by a spring. The kinetic energy function is

$$K(\phi, \dot{\phi}) = \frac{1}{2} \sum_{j=1}^l m_j \dot{\phi}_j^2$$

and the Lagrangian of the system is $L(\phi, \dot{\phi}) = K(\phi, \dot{\phi}) - U(\phi)$. We refer to the β_{ij} also as the *spring constants*.

Exercise 2.6. Show that the Euler-Lagrange equations $\frac{d}{dt} \frac{\partial L}{\partial \dot{\phi}_j} - \frac{\partial L}{\partial \phi_j} = 0$ for the spring-mass network is

$$m_i \ddot{\phi}_i + \sum_{r \neq i} \beta_{ri} (\phi_i - \phi_r) = 0$$

for $i = 1, \dots, l$. Write down in detail the equations and boundary conditions for the example of Figure 8. Assume all the β_{ij} are equal and that the boundary function f is identically 0.

It is illuminating to look at the spring-mass network in a more abstract way that makes it formally related (as a graph counterpart) to the continuum wave equation. For the sake of this discussion a *graph* will be understood as a pair of sets $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ where \mathcal{V} is called the set of *vertices* and \mathcal{E} the set of *edges*. We assume that \mathcal{V} is a finite set and that \mathcal{E} consists of ordered pairs of distinct vertices, $\mathcal{E} \subset \mathcal{V} \times \mathcal{V}$. If $(u, v) \in \mathcal{E}$ we write $u \sim v$ and when the direction of $e \in \mathcal{E}$ becomes important we write $e = (e^-, e^+)$. We assume, nevertheless, that the graph is essentially not directed, in the sense that if $e = (e^-, e^+) \in \mathcal{E}$ then also $\bar{e} := (e^+, e^-) \in \mathcal{E}$. The masses m_j and spring constants (by which we now mean the β_{ij} rather than the k_{ij}) are viewed as functions on the sets of vertices and edges, respectively. Thus $m : \mathcal{V} \rightarrow (0, \infty)$ and $\beta : \mathcal{E} \rightarrow (0, \infty)$, where $\beta(u, v) = \beta(v, u)$ for all $u \sim v$. Let $L^2(\mathcal{V}, m)$ denote the vector space of complex valued functions on \mathcal{V} endowed with the inner product

$$\langle \varphi, \psi \rangle := \sum_{v \in \mathcal{V}} \varphi(v) \overline{\psi(v)} m(v).$$

The *Laplace operator* or *Laplacian* associated to (\mathcal{G}, m, β) is the linear operator on $L^2(\mathcal{V}, m)$ defined by

$$(\mathcal{L}\varphi)(v) := \sum_{w \sim v} \frac{\beta(v, w)}{m(v)} (\varphi(w) - \varphi(v)).$$

Allowing functions to also depend on time, $t \mapsto \varphi(\cdot, t) \in L^2(\mathcal{V}, m)$, then φ represents the motion of a spring-mass network if it satisfies the discrete wave equation

$$\frac{d^2 \varphi}{dt^2} + \mathcal{L}\varphi = 0.$$

Exercise 2.7 (The graph Laplacian is self-adjoint). Prove that \mathcal{L} is a self-adjoint linear operator on $L^2(\mathcal{V}, m)$. That is, show that $\langle \mathcal{L}\varphi, \psi \rangle = \langle \varphi, \mathcal{L}\psi \rangle$ for all $\varphi, \psi \in L^2(\mathcal{V}, m)$. In particular, the eigenvalues of \mathcal{L} are real and it can be diagonalized using an orthonormal basis of eigenvectors.

It turns out that \mathcal{L} is non-positive definite, that is, its eigenvalues are non-positive real numbers. This will follow from the observation that it is possible to define operators d and its adjoint d^* so that $\mathcal{L} = -d^*d$, which should be compared with the expression of the continuous Laplacian as the composition of div and grad. But first we define another vector space of functions, now on \mathcal{E} . This is the linear space (over \mathbb{C}) denoted $L^2(\mathcal{E}, 1/\beta)$ consisting of complex valued functions X on \mathcal{E} such that $X(\bar{e}) = -X(e)$ for all $e \in \mathcal{E}$, where $(e^-, e^+) = (e^+, e^-)$, and endowed with the inner product

$$\langle X, Y \rangle := \frac{1}{2} \sum_{e \in \mathcal{E}} X(e) \overline{Y(e)} \beta(e)^{-1}.$$

It makes sense to think of X and Y as vector fields on the graph.

The graph *gradient* operator is the linear operator $\mathcal{D} : L^2(\mathcal{V}, m) \rightarrow L^2(\mathcal{E}, 1/\beta)$ defined by

$$(\mathcal{D}\varphi)(e) := [\varphi(e^+) - \varphi(e^-)]\beta(e).$$

Also define the (minus) *divergence* operator $\mathcal{D}^* : L^2(\mathcal{E}, 1/\beta) \rightarrow \mathcal{D} : L^2(\mathcal{V}, m)$ by

$$(\mathcal{D}^* X)(v) := \frac{1}{m(v)} \left(\sum_{e^+=v} X(e) - \sum_{e^-=v} X(e) \right).$$

The norms derived from the inner products on the vector spaces of functions and vector fields on \mathcal{G} will both be denoted by $\|\cdot\|$.

Exercise 2.8 (Properties of grad, div, and the Laplacian). Prove the following properties.

1. \mathcal{D}^* is the adjoint operator of \mathcal{D} . That is, for all $X \in L^2(\mathcal{E}, 1/\beta)$ and all $\varphi \in L^2(\mathcal{V}, m)$,

$$\langle \mathcal{D}^* X, \varphi \rangle = \langle X, \mathcal{D}\varphi \rangle.$$

2. We have $\mathcal{L}\varphi = -\mathcal{D}^* \mathcal{D}\varphi$ for all $\varphi \in L^2(\mathcal{V}, m)$.

3. The eigenvalues of \mathcal{L} are all non-positive.

4. For all $\varphi \in L^2(\mathcal{V}, m)$,

$$\|\mathcal{D}\varphi\|^2 \leq \sup_{v \in \mathcal{V}} \left(\frac{1}{m(v)} \sum_{u: (u,v) \in \mathcal{E}} \beta(u, v) \right) \|\varphi\|^2.$$

5. Let $\{\varphi_1, \dots, \varphi_N\}$ be an orthonormal basis of $L^2(\mathcal{V}, m)$ consisting of eigenvectors of \mathcal{L} . Show that

$$\varphi(v, t) = \sum_{j=1}^N c_j e^{\sqrt{\lambda_j} t} \varphi_j(v)$$

is the unique solution of the wave equation $\ddot{\varphi} + \mathcal{L}\varphi = 0$ with initial condition

$$\varphi(v, 0) = \sum_{j=1}^N c_j \varphi_j(v).$$

Note that the exponentials tend to produce oscillatory behavior since $\lambda_j \leq 0$.

add boundary conditions

2.4 SYSTEMS WITH COLLISIONS

Mechanical systems on configuration manifolds with boundary, or more generally corners, are interesting in that boundary configurations represent collisions between constituent parts of the system. In this section we discuss in some detail one of the simplest examples of this kind, shown in Figure 9, which will be used to introduced some elementary but useful ideas.

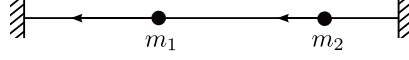


Figure 9: Two point masses can slide freely on an interval. They collide elastically with each other and with the fixed walls at the endpoints of the interval. We assume that interval has length L .

The material body in this case consists of two points, which we identify with the indices of the masses, $\mathcal{B} = \{1, 2\}$, and the mass distribution measure μ is simply $\mu(i) = m_i$, $i = 1, 2$. The manifold of configuration is the set

$$M = \{q = (x_1, x_2) \in [0, L] \times [0, L] : x_1 \leq x_2\}$$

which is a manifold with corners. Here L is the length of the interval. The position map is simply $\Phi(x, i) = x_i$. The kinetic energy Riemannian metric is given by

$$\langle u, v \rangle = m_1 u_1 v_1 + m_2 u_2 v_2$$

and the kinetic energy is $K(q, v) = \frac{1}{2} \|v\|^2$ where $\|\cdot\|$ is the norm associated to this Riemannian metric. Clearly, geodesics in this metric are the same as for the Euclidean metric on the plane, so the dynamic in the interior of M is described by uniform rectilinear motion.

Further assumptions about the nature of contact between the point masses and between each point mass and the walls are needed in order to determine the motion after a trajectory hits the boundary of M . A natural choice, which we make here, is to impose the conditions that the total energy and linear momentum do not change. So let q be a boundary point in M and denote by v^- and v^+ the velocities of a trajectory in M before and after, respectively, it hits the boundary at q . We first consider the case of a collision between the two point masses. First note that $\tau = (1, 1)/\sqrt{m_1 + m_2}$ is a unit vector (in the kinetic energy metric) tangent to the diagonal boundary component $x_1 = x_2$. The momentum associated to a velocity v at q is

$$m_1 v_1 + m_2 v_2 = m^{1/2} \langle v, \tau \rangle$$

where $m := m_1 + m_2$. Therefore, conservation of momentum in a collision between the points masses can be expressed by saying that the component of the velocity tangential to the boundary at q must remain invariant. Energy conservation, interpreted in terms of the kinetic energy metric, means that the length of the velocity vector is also invariant. This means that the velocity v^+ after collision is the mirror reflection of the velocity v^- before collision on the boundary of M . A similar but simpler argument applies to collisions of each point mass with the ends of the interval, if we imagine those ends as being walls of infinite mass and the collisions energy preserving.

Proposition 2.1 summarizes the foregoing discussion. The term *elastic collision* will be used to indicate that the assumptions made above about energy and momentum conservation at collisions are in place.

Proposition 2.1. Relative to the kinetic energy (Euclidean) Riemannian metric on the configuration space M , the motion of the two point masses system, with masses m_1 and m_2 and with elastic collisions, corresponds to billiard motion (with specular reflection at the boundary) on a right triangle shaped billiard table. The angle θ at one of the two vertices contained in the hypotenuse satisfies $\tan \theta = \sqrt{m_1/m_2}$.

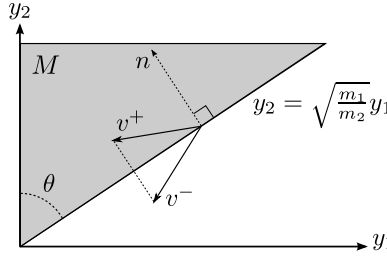


Figure 10: The configuration manifold of the two particles system described in terms of the kinetic energy Riemannian metric. Dynamics correspond to ordinary billiard motion in a right-triangle whose shape is determined by the ratio of the two masses.

An alternative way to describe the conclusion of Proposition 2.1 is as follows. Introduce a new system of coordinates in \mathbb{R}^2 by the expression $y_i = (m_i/m)^{1/2} x_i/l$, $i = 1, 2$. In the new system, the kinetic energy of a state $((y_1, y_2), (\dot{y}_1, \dot{y}_2))$ assumes the form $ml^2(\dot{y}_1^2 + \dot{y}_2^2)$ and energy is now proportional to Euclidean length. In this new coordinate system motion of the two-particle system is as described in the proposition. While the triangle was isosceles in the (x_1, x_2) -coordinates, in the new metric *pulled-back* under the coordinate change the sides of the triangle adjacent to the right angle have lengths $\sqrt{m_i/m}$, $i = 1, 2$. (By the choices made, lengths in the new coordinates (y_1, y_2) have been rendered *dimensionless* in the sense that they are free of physical units.)

Exercise 2.9. Consider the motion of two point masses on the half-infinite line as shown in Figure 11. We suppose that the point mass m_2 starts at a point x_2 with velocity $v_2 < 0$ and that

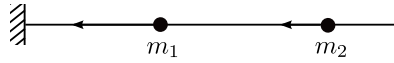


Figure 11: Two masses system in a half-infinite interval.

m_1 starts with velocity v_1 . After a certain number n_c of collisions between the two masses and between m_1 and the left wall, m_2 reverses direction and moves back towards the right end of the interval, never again to hit m_1 . Show that the total number n_c of collisions can be bounded

from above by

$$n_c \leq \left\lceil \left(\arctan \sqrt{\frac{m_1}{m_2}} \right)^{-1} \pi \right\rceil$$

Where $\lceil x \rceil$ denotes the least integer greater than or equal to x . (Suggestion: Consider the wedge shaped billiard table obtained in the way we did for the triangle of Proposition 2.1 then “unfold” it as shown in Figure 12.)

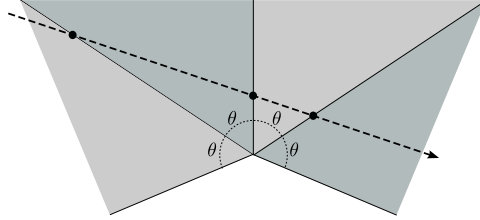


Figure 12: The *unfolding* method used in Exercise 2.9.

In Exercise 2.9 you have used the idea of investigating a property of billiard trajectories by the method of unfolding the billiard table, whereby the polygonal trajectories become straight lines. We now explore this simple but useful idea a bit further. We want to show that, when $\sqrt{m_1/m_2}$ is the tangent of an angle of the form $\pi p/q$, where p, q are positive integers, then a minimal unfolding of the triangular billiard table of Proposition 2.1 can be obtained by gluing a number of copies of the table, resulting in a flat closed surface with singularities, on which motion becomes rectilinear and uniform. For more details on the relationship between billiard dynamics and complex function theory we recommend [6].

Let us consider the simple example of a rectangular billiard table before tackling the general case of polygonal tables. The unfolding procedure is explained in Figure 13.

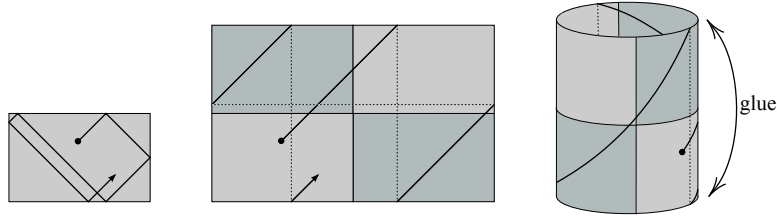


Figure 13: The unfolding of a rectangular billiard table results in a flat torus in which billiard motion is geodesic. The four copies of the original table are at glued together at their common edges in such a way that adjacent pairs are mirror images of each other, producing a rectangle four times larger in area. The two parallel pairs of sides of this larger rectangle are then glued together to form a torus.

We now consider a general polygonal billiard table M . The goal is to construct a flat surface without boundary on which trajectories of the billiard system are geodesic paths. We wish the resulting surface to be, in some sense, minimal in size. Note, for example, that for the rectangular table of Figure 13 we could have kept reflecting copies of the rectangle at their sides indefinitely so as to produce a tiling of the entire plane instead of the torus we actually obtained. Similarly for M , we want as few reflected copies as possible produce a closed surface without boundary. We will see that when M is a rational polygon (see Figure 14) the result of the unfolding is a closed surface of finite area without boundary with a number of singular points and genus that can be computed from the values of the corner angles.

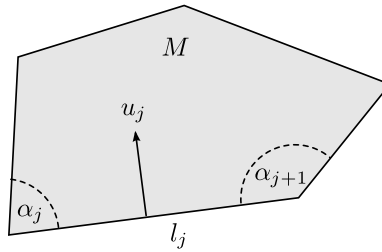


Figure 14: A polygonal billiard table. The inward pointing unit normal vector to side l_j is u_j . The polygon is said to be *rational* if the angle at each vertex is a rational multiple of π , that is, $\alpha_j = \pi p_j / q_j$ for each j .

Exercise 2.10 (Reflection groups). To each side l_j , $j = 1, \dots, m$, of the polygon of Figure 14 we associate the linear transformation of \mathbb{R}^2 defined by $R_j x = x - 2\langle x, u_j \rangle u_j$ where u_j is the inward pointing unit normal vector to l_j and $\langle x, u_j \rangle u_j$ denotes the standard inner product

(dot product) on \mathbb{R}^2 . The *reflection maps* R_j together generate a subgroup G of the group of orthogonal transformations

$$O(2) = \{A : \text{two-by-two real matrix such that } A^\dagger A = I\}.$$

Assume that the *reflection group* G is a finite group. Show the following.

1. $\alpha_j = \pi p_j / q_j$ for each j , where p_j and q_j are positive coprime numbers.
2. G is a dihedral group of order $2N$, where N is the least common multiple of $\{q_1, \dots, q_m\}$.
3. $G = H \cup R_1 H$, a union of disjoint sets where H is a cyclic group consisting of rotation matrices, that is, matrices in $O(2)$ having determinant 1.

Note: For basic facts concerning reflection groups see [4].

A *billiard dynamical system* on a planar billiard table in dimension 2 is a mechanical system whose configuration manifold is a region of \mathbb{R}^2 with piecewise smooth boundary, and kinetic energy Riemannian metric given by ordinary dot product. Trajectories describe rectilinear uniform motion in the interior of M with specular reflection at boundary points. Since the length of vectors are unchanged during motion (energy conservation) it makes sense to restrict attention to the submanifold V of TM consisting of unit vectors. We call V the (restricted) *phase space* of the billiard. Clearly, $V = M \times S^1$, where S^1 is the set of unit vectors in \mathbb{R}^2 . Alternatively, we may use the angle of a vector relative to a fixed basis of \mathbb{R}^2 to represent a state in V , in which case the circle S^1 is identified with the set of angles $\theta \pmod{2\pi} \in \mathbb{R}/(2\pi\mathbb{Z})$.

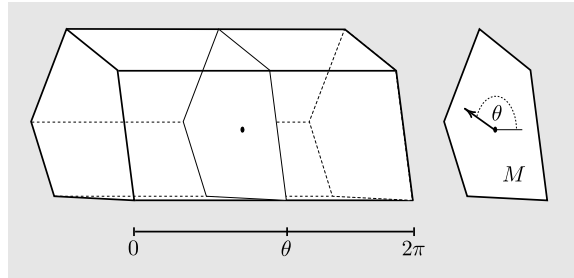


Figure 15: The space of unit length velocities of the billiard system is the product $V = M \times \mathbb{R}/(2\pi\mathbb{Z})$. A point in the θ -labeled slice represents a velocity at the projected point on M in the direction of angle θ relative to a fixed frame. The two faces at 0 and 2π are identified, resulting in a solid torus.

Observe that the group G generated by reflections on the sides of the billiard table (whether or not M is a rational polygon) acts on S^1 by linear transformations. This linear action induces an action of G on the boundary of V , which we write $(q, v) \mapsto (q, R_j v)$ where q is in the boundary of M , v is a unit vector, and R_j is a generator of G .

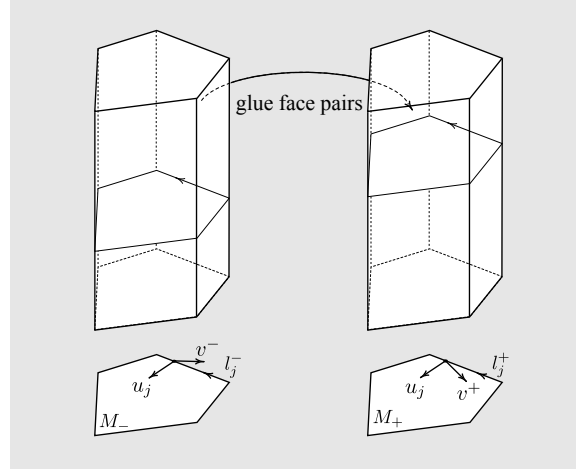


Figure 16: Unfolded billiard phase space. Two copies V^- and V^+ of the prism of Figure 15 are glued along the pairs of faces $l_j^- \times S^1$, $l_j^+ \times S^1$. The gluing maps are $(q, v^-) \mapsto (q, v^+)$, where $v^+ = R_j v^-$ and R_j is reflection on l_j . Thus the plaque at level θ^- of V^- is glued to the plaque at level θ^+ along the common side l_j , where θ and θ' are the angles parametrizing v^- , v^+ relative to a choice of basis in \mathbb{R}^2 .

By using the idea of unfolding we can extend the billiard motion to an enlarged phase space without boundary, in which trajectories become rectilinear paths. The main idea is described in Figure 16.

We take two copies of the billiard phase space (the prism of Figure 15), which we denote by V^- and V^+ . The *unfolded phase space* is defined as the quotient $W = (V^- \cup V^+) / \sim$ in which \cup indicates disjoint union and \sim is the equivalence relation defined as follows. If one or both of q, q' are interior points of M , then $(q, v) \sim (q', v')$ if and only if $(q, v) = (q', v')$. If both q and q' are boundary points, then $(q, v) \sim (q', v')$ if and only if $q = q'$, q lies on side l_j for some j , and $v' = R_j v$. Note that $R_j^2 = I$, so $v' = R_j v$ if and only if $v = R_j v'$. Thus quotient space W is obtained by gluing the pairs of faces V_j^-, V_j^+ , where $V_j^\pm = l_j^\pm \times S^1$ and l_j^\pm are two copies of l_j . For each corner vertex q_j of M let S_j denote the circle $\{q_j\} \times S^1$.

Exercise 2.11. The unfolded phase space W associated to the polygonal billiard table M is a compact, Hausdorff topological space. The open subset $W_0 := W \setminus \bigcup_j S_j$ is a smooth 3-dimensional manifold foliated by smooth, flat, oriented surfaces. Representing a point in W by $[q, v]$, the rotation group $SO(2)$ acts on W continuously by $(g, [q, v]) \mapsto [q, gv]$, and smoothly on the invariant subset W_0 , respecting the foliation, that is, mapping each leaf into another leaf diffeomorphically. (That the leaves have a flat structure can be interpreted as saying that for a natural choice of atlas, on the overlap of two foliated charts of W_0 , the change of coordinates mapping, defined between open subsets of $\mathbb{R}^2 \times \mathbb{R}$, restricts to affine maps on \mathbb{R}^2 .) Each leaf of the (singular) foliation of W by flat surfaces is the image into W of the union $\bigcup_{g \in G} (M \times \{gv\})$

for some $v \in S^1$. We denote the leaf through (q, v) by $\mathcal{S}(v)$, or simply by \mathcal{S} as the leaves through different v are essentially the same.

When the reflection group G generated by the R_j is finite, the unfolded phase space becomes foliated by closed (compact, boundariless) flat surfaces, denoted \mathcal{S} in Exercise 2.11, that are permuted among themselves by translations in the angle θ . Let us now assume that G is finite, hence the table M is a rational polygon according to Exercise 2.10, and try to determine how \mathcal{S} looks like.

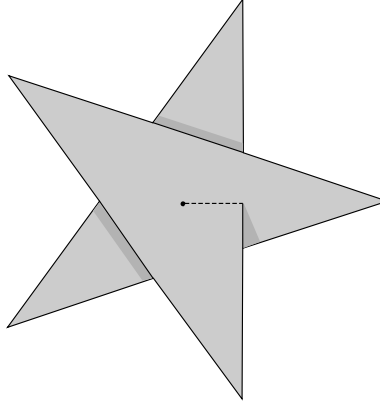


Figure 17: The angle at a singular point of the unfolded polygon is by definition the length of the circumference divided by the radius of a small circle centered at the point. For this star shaped region, the singular point at the center has angle 4π .

Proposition 2.2 (Topology of the unfolded billiard table). Let M be a rational polygon with m sides and inner angles $\alpha_j = \pi p_j / q_j$, $j = 1, \dots, m$, where p_j, q_j are coprimes. (See Figure 14.) Let G be the finite reflection group generated by the reflections on the m sides and \mathcal{S} the surface constructed by unfolding M . Then \mathcal{S} is an orientable surface without boundary with area equal to $2N \times \text{Area}(M)$, where N is the least common multiple of q_1, \dots, q_m . The tiling of \mathcal{S} by copies of M gives \mathcal{S} a polygonal decomposition with $2N$ faces, mN edges, and $N \sum_{j=1}^m 1/q_j$ vertices, thus with Euler characteristics

$$\chi(\mathcal{S}) = N \left(\sum_{j=1}^m \frac{1}{q_j} - m + 2 \right) = N \sum_{j=1}^m \frac{1 - p_j}{q_j}$$

where the number of sides is $m = 2 + \sum_{j=1}^m p_j / q_j$. The complement of the vertices in \mathcal{S} has the structure of a smooth flat surface, whereas for each j and each u among the N/q_j vertices corresponding to angle α_j , the angle at u is $2\pi p_j$. (See Figure 17.) In particular \mathcal{S} has genus $g = 1 + (N/2) \sum_{j=1}^m (p_j - 1)/q_j$.

Proof. *

□

Exercise 2.12. Consider a mechanical system of the type described at the beginning of this section, consisting of two masses of values m_1 and m_2 in an interval. Suppose that the ratio of masses is $m_1/m_2 = 3 - \sqrt{2}$, so that $\sqrt{m_1/m_2} = \tan \pi/8$. Then the mechanical system corresponds to a billiard system on a table in the shape of a right triangle having one inner angle equal to $\pi/8$. Show that the unfolded table is a flat surface of genus 2 with one singular point with angle 6π .

2.5 MORE EXAMPLES OF BILLIARD-LIKE SYSTEMS

3 MECHANICAL SYSTEMS AND RIEMANNIAN GEOMETRY

We want here to provide some perspective into what we have discussed so far by describing Newtonian systems in differential geometric terms. This section assumes some acquaintance with the basic definitions and facts from Riemannian geometry, although we will try to make it reasonably self-contained. The first few chapters of [1] are sufficient for our needs. A smooth manifold M will represent the configuration space of a mechanical system having kinetic energy function $K(q, v) = \frac{1}{2} \|v\|_q^2$, where $\|v\|_q^2 = \langle v, v \rangle_q$, and $q \mapsto \langle \cdot, \cdot \rangle_q$ is the Riemannian metric, which is a smooth field of symmetric, non-degenerate bilinear forms on the tangent bundle TM . We say that a mechanical system with configuration manifold M is *Newtonian* if its Lagrangian function $L : TM \rightarrow \mathbb{R}$ has the expression

$$L(q, v) = K(q, v) - U(q)$$

where $U(q)$ is a potential function.

3.1 MOTION CONSTRAINED TO SUBMANIFOLDS OF \mathbb{R}^N

We have so far expressed the Euler-Lagrange equations in a fixed coordinate system. It is often desirable to have a more intrinsic, coordinate-free expression of the equations of motion of a mechanical system, something we will obtain shortly for a general Newtonian system. In this subsection we consider the special case of a particle of mass m in \mathbb{R}^N that is constrained to move in a submanifold M of dimension $n < N$. An example to keep in mind is a pendulum in \mathbb{R}^3 with the pivot at the origin and rod of a fixed length r , in which case the bob is restricted to move on a 2 dimensional sphere of radius r .

The definitions of Lagrangian function, action, variation, and critical path are those of Section 2.2, now applied to the configuration manifold M . (The formal setting could be, trivially, $\mathcal{B} = \{0\}$, mass distribution measure $\mu(0) = m$, and position map $\Phi(q, 0) = q$.) The equations of motion are, as before, derived from Hamilton's principle of stationary action.

Exercise 3.1 (The Euler-Lagrange equations with constraints on position). Using the same argument of Theorem 2.1 in the standard coordinates $q = (q_1, \dots, q_N)$ of \mathbb{R}^N , show that a path $\gamma : [a, b] \rightarrow M$ is L -critical for the Lagrangian function $L(q, v)$ restricted to $(q, v) \in TM$ if and only if the vector field $X(t) = (X_1(t), \dots, X_N(t))$ defined along the path $\gamma(t)$ by

$$X_j := \frac{\partial L}{\partial q_j} - \frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{q}_j} \right)$$

is perpendicular to TM for all t .

We now apply the result of Exercise 3.1 to a Newtonian Lagrangian $L(q, v) = \frac{1}{2} m \|v\|^2 - U(q)$. Let Π_q denote the orthogonal projection from \mathbb{R}^N onto $T_q M$, where the latter is regarded as a linear subspace of \mathbb{R}^N . Then a path $\gamma(t)$ on M is L -critical if and only if $\Pi_{\gamma(t)} X(t) = 0$ for all t , where $X(t) = -\text{grad}_{\gamma(t)} U - \gamma''(t)$. So the equation of motion is

$$\Pi_{\gamma(t)} [\gamma''(t) + \text{grad}_{\gamma(t)} U] = 0.$$

In particular, in the absence of potential forces, the equation reduces to $\Pi_{\gamma(t)}\gamma''(t) = 0$.

Exercise 3.2. Show that the following are equivalent for a smooth path $\gamma : \mathbb{R} \rightarrow \{x \in \mathbb{R}^3 : \|x\| = r\}$.

1. $\Pi_{\gamma(t)}\gamma''(t) = 0$
2. $\gamma''(t) + \omega\gamma(t) = 0$ for some $\omega \in \mathbb{R}$
3. $\gamma(t) = \gamma(0)\cos(\omega t) + \frac{1}{\omega}\gamma'(0)\sin(\omega t)$.

Note: (1) implies that $\gamma''(t) = f(t)\gamma(t)$ for some smooth function $f(t)$, so to prove (2) from (1) it is necessary to show that $f'(t) = 0$. For this, start with the equation $\|\gamma(t)\|^2 = r^2$ and take successive derivatives. The first derivative gives $\langle \gamma'(t), \gamma(t) \rangle = 0$.

4 RIGID MOTIONS IN EUCLIDEAN SPACE

4.1 EUCLIDEAN ISOMETRIES AND THE GROUPS $E(n)$ AND $SE(n)$

An important role is played in classical mechanics by the group of rigid motions in Euclidean space. It is clearly needed, for example, in the description of the motion of rigid bodies. Consider the motion of a solid body \mathcal{B} in \mathbb{R}^3 . Here $\mathcal{B} \subset \mathbb{R}^3$ is the body in a fixed, reference configuration. Any other configuration of \mathcal{B} is described by a mapping $\sigma : \mathcal{B} \rightarrow \mathbb{R}^3$ (say, smooth, invertible on its image, orientation preserving). Given $x \in \mathcal{B}$, the image $\sigma(x)$ is the location in space occupied by the material point x . We say that \mathcal{B} is a *rigid body* if its configurations are orientation preserving isometries of \mathbb{R}^3 .

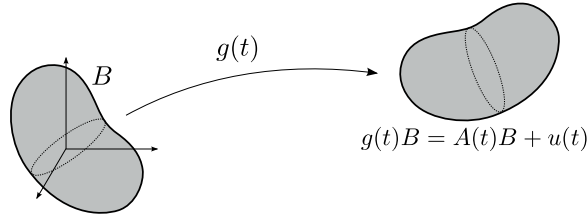


Figure 18: The motion of a rigid body in 3-space is described by a path in $SE(3)$.

In this section, we take some time to familiarize ourselves with the group of isometries of Euclidean space. Let $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ be a diffeomorphism of \mathbb{R}^n , that is, an invertible everywhere differentiable map whose inverse is also everywhere differentiable. We say that f is an *isometry* from a non-empty open subset U of \mathbb{R}^n into \mathbb{R}^n if for any two points $x, y \in U$,

$$\text{dist}(f(x), f(y)) = \text{dist}(x, y),$$

where $\text{dist}(x, y) := |x - y|$ is the Euclidean distance between x and y . We show next that any isometries in \mathbb{R}^n is the restriction to U of an affine map (i.e., a linear map composed with a translation) whose linear part is in the *orthogonal group*

$$O(n) := \{A \text{ an } n\text{-by-}n \text{ real matrix} : A^\dagger A = I\}.$$

But first observe the following.

Proposition 4.1. A real n -by- n matrix A belongs to the orthogonal group $O(n)$ if and only if $|Au| = |u|$ for all $u \in \mathbb{R}^n$.

Proof. Recall that the transpose A^\dagger is the matrix related to A by the identity $\langle A^\dagger u, v \rangle = \langle u, Av \rangle$ for all $u, v \in \mathbb{R}^n$. Hence the condition $A^\dagger A = I$ is exactly equivalent to $\langle Au, Av \rangle = \langle u, v \rangle$ for all u, v . Clearly, if A respects the Euclidean inner product, it leaves the Euclidean norm invariant. Conversely, if A leaves invariant the Euclidean norm,

$$|u + v|^2 = |A(u + v)|^2 = |Au|^2 + |Av|^2 + 2\langle Au, Av \rangle = |u|^2 + |v|^2 + 2\langle u, v \rangle$$

from which it follows that $\langle Au, Av \rangle = \langle u, v \rangle$ for all u, v . \square

Proposition 4.2. Let U be a non-empty open set of \mathbb{R}^n . Then for all $x \in U$, the differential df_x of an isometry $f : U \rightarrow \mathbb{R}^n$ is an element of $O(n)$.

Proof. Note the following:

$$\begin{aligned} |df_x u| &= \left| \lim_{h \rightarrow 0} \frac{f(x + hu) - f(x)}{h} \right| \\ &= \lim_{h \rightarrow 0} \left| \frac{f(x + hu) - f(x)}{h} \right| \\ &= \lim_{h \rightarrow 0} \frac{|f(x + hu) - f(x)|}{|h|} \\ &= \lim_{h \rightarrow 0} \frac{|x + hu - x|}{|h|} \\ &= |u|. \end{aligned}$$

Therefore, df_x is an orthogonal transformation by Proposition 4.1. \square

We conclude:

Theorem 4.1. Any isometry $f : U \rightarrow \mathbb{R}^n$, where U is a nonempty open set in \mathbb{R}^n , has the form

$$f(x) = f(0) + Ax,$$

where A is an element of $O(n)$.

Proof. Without loss of generality we may assume that $0 \in U$. Otherwise we simply translate U by $-x_0$ for some x_0 in U , keeping in mind that the composition of two isometries is also an isometry. Define the transformation $T(x) = A^{-1}(f(x) - f(0))$ where $A = df_0$. Then T is an isometry that fixes 0 and $dT_0 = I$. We wish to conclude that T is the identity map.

Define the smooth path $\gamma(t) = T(tu)$, for any vector u so that that tu lies in U for all $0 \leq t \leq 1$. Then $\gamma(0) = 0$ and $\gamma'(0) = u$. As dT_x is orthogonal by Proposition 4.2,

$$L(t) = \text{length of } \gamma|_{[0,t]} = \int_0^t |\gamma'(s)| ds = \int_0^t |dT_{su} u| ds = \int_0^t ds = t|u| = |tT(u)|.$$

This means that both the smooth path $t \mapsto T(tu)$ and the straight line $t \mapsto tT(u)$, $0 \leq t \leq 1$, have the same length and connect 0 to u . We now define $v(t) := T(tu)/|T(tu)|$ and observe that $\gamma(t) = t|u|v(t)$, since $|T(tu)| = t|u|$. Being a smooth vector-value function of unit norm for all t , $v(t)$ satisfies $\langle v'(t), v(t) \rangle = 0$. This implies that

$$|\gamma'(t)| = ||u|v(t) + t|u|v'(t)| = |u|(1 + t^2|v'(t)|^2)^{1/2}.$$

Integrating from 0 to 1 gives

$$|u| = \text{length of } \gamma|_{[0,1]} = |u| \int_0^1 \sqrt{1 + t^2|v'(t)|^2} dt \geq |u|.$$

The conclusion is that $v'(t)$ should vanish identically, so $T(tu) = tw$ for a constant vector w . Taking the derivative in t at $t = 0$ yields $w = dT_0 u = u$. Therefore, $T(tu) = tu$ for all $t \in [0, 1]$ and u small enough. In other words, T is the identity map in a neighborhood of 0. As noted at the beginning, this conclusion holds at any $x \in U$, so T is the identity map on all of U and $f(x)$ is as stated. \square

Definition 4.1 (The Euclidean group). The set of all isometries of \mathbb{R}^n , which consists of all the affine maps of the form $x \mapsto Ax + a$ for $A \in O(n)$ and $a \in \mathbb{R}^n$, is called the *Euclidean group*, or the group of *Euclidean motions* of \mathbb{R}^n , denoted $E(n)$. The orientation preserving Euclidean motions constitutes the subgroup $SE(n)$, whose elements have the form $Ax \mapsto x + a$ for $A \in SO(n)$, where $SO(n)$ is the group of orthogonal matrices of determinant 1.

Exercise 4.1. Verify that $E(n)$ is indeed a group under composition and that it is isomorphic to the semidirect product $O(n) \ltimes \mathbb{R}^n$. The latter is defined as the product $O(n) \times \mathbb{R}^n$ with multiplication

$$(A_2, a_2)(A_1, a_1) = (A_2 A_1, A_2 a_1 + a_2).$$

Determine the expression for the inverse of (A, a) .

Exercise 4.2. Let $GL(n+1, \mathbb{R})$ denote the *general linear group* in dimension $n+1$, which by definition consists of all the invertible real matrices of size $(n+1)$ -by- $(n+1)$. Show that $E(n)$ can be viewed as a subgroup of $GL(n+1, \mathbb{R})$ under the correspondence:

$$(A, u) \in O(n) \ltimes \mathbb{R}^n \mapsto \begin{pmatrix} A & u \\ 0 & 1 \end{pmatrix} \in GL(n+1, \mathbb{R}).$$

4.2 THE LIE ALGEBRA OF INFINITESIMAL EUCLIDEAN MOTIONS

The Lie algebra $\mathfrak{se}(n)$ of $SE(n)$ consists of the matrices $\begin{pmatrix} X & w \\ 0 & 0 \end{pmatrix} \in M_{n+1}(\mathbb{R})$ where $X \in \mathfrak{so}(n)$ is a skew-symmetric matrix and w is any vector in \mathbb{R}^n .

Exercise 4.3. Show that one-parameter subgroups of $SE(n)$ have the form

$$\sigma(t) := \exp \left(t \begin{pmatrix} X & w \\ 0 & 0 \end{pmatrix} \right) = \begin{pmatrix} e^{tX} & (\int_0^t e^{sX} ds) w \\ 0 & 1 \end{pmatrix}.$$

Check by direct computation that $\sigma(t_1 + t_2) = \sigma(t_1)\sigma(t_2)$.

We wish next to discuss in some detail the situation in dimension 3. Recall that the *cross-product* on \mathbb{R}^3 is the (nonassociative, noncommutative) multiplications defined by

$$(a_1, a_2, a_3) \times (b_1, b_2, b_3) = (a_2 b_3 - b_2 a_3, a_3 b_1 - a_1 b_3, a_1 b_2 - b_1 a_2).$$

Now, for each $a = (a_1, a_2, a_3) \in \mathbb{R}^3$, define $\omega(a) \in M(3, \mathbb{R})$ by $\omega(a)b := a \times b$, where b is a column vector in \mathbb{R}^3 . Thus $\omega(a)$ is the matrix of the linear map $b \mapsto a \times b$.

Exercise 4.4. Show that $(\mathbb{R}^3, [\cdot, \cdot])$, with bracket $[a, b] := a \times b$, is a Lie algebra isomorphic to $\mathfrak{so}(3)$. Show this by proving that $\omega(a \times b) = [\omega(a), \omega(b)]$, where the bracket on the right-hand side is the commutator of matrices. In particular, cross-product satisfies the Jacobi identity

$$a \times (b \times c) + b \times (c \times a) + c \times (a \times b) = 0.$$

Exercise 4.5. For all $a, b \in \mathbb{R}^3$, show that

$$e^{\omega(a)} b = b + (a \times b) \sin \theta + (\langle a, b \rangle a - |a|^2 b)(1 - \cos \theta).$$

This is obtained from $e^{\theta \omega(a)} = \sum_{n=0}^{\infty} \frac{\theta^n}{n!} \omega(a)^n$ by first proving the identities:

$$\omega(a)^2 b = \langle a, b \rangle a - |a|^2 b, \quad \omega(a)^3 b = -|a|^2 \omega(a) b.$$

Exercise 4.6. Let a, b, c be unit vectors in \mathbb{R}^3 forming a positive orthonormal basis and write $R(a, \theta) := e^{\theta \omega(a)}$, which is a one parameter subgroup of $SO(3)$. Show that

1. $R(a, \theta)a = a$
2. $R(\theta, a)b = b \cos \theta + c \sin \theta$.

Conclude that $R(\theta, a)$ is a rotation by θ about the axis determined by a .

Exercise 4.7. Show that for any $S \in SO(3)$, $a, b \in \mathbb{R}^3$, and $\theta \in \mathbb{R}$,

1. $R(\theta, Sa) = SR(\theta, a)S^{-1}$
2. $S(a \times b) = Sa \times Sb$.

Elements of $\mathfrak{so}(3)$ have been shown to take the form $\theta \omega(a)$, $|a| = 1$. The next proposition says that every element of $SO(3)$ can be written as $R(\theta, a)$ for some θ and a . In particular, every element of $SO(3)$ is a rotation about some axis (one-dimensional subspace) in \mathbb{R}^3 .

Proposition 4.3. The exponential map $\exp : \mathfrak{so}(3) \rightarrow SO(3)$, $\exp(A) := e^A$, is surjective.

Proof. Let $S \in SO(3)$. We claim that 1 is an eigenvalue of S . Note that S has a nonzero real eigenvalue λ , since its characteristic polynomial has degree 3. Let a be a unit eigenvector associated to λ . Since $\lambda^2 |a|^2 = \langle Sa, Sa \rangle = |a|^2$, λ must be either 1 or -1 . If the other eigenvalues are nonreal, then we have two complex conjugate eigenvalues, μ and $\bar{\mu}$, so that $1 = \det(A) = \lambda \mu \bar{\mu} = \lambda |\mu|^2$, from which we deduce that $\lambda = 1$. Notice that S restricts to an orthogonal transformation on the plane a^\perp perpendicular to a . If the transformation $S|_{a^\perp}$ has one real eigenvalue with unit eigenvector b , then a unit vector perpendicular to both a and b will also be an eigenvector.

Therefore, if $\lambda = -1$, S is diagonalizable with real eigenvalues, which are all either 1 or -1 . But the product of the eigenvalues is 1, so at least one of them must be 1 as claimed. Let a be a unit eigenvector with eigenvalue 1. Let b and c be unit vectors such that $\langle a, b, c \rangle$ forms a positive orthogonal basis of \mathbb{R}^3 . Then $Sb = \alpha b + \beta c$, where α and β are real numbers such that $\alpha^2 + \beta^2 = 1$. Therefore, there is $\theta \in \mathbb{R}$ such that $\alpha = \cos \theta$ and $\beta = \sin \theta$. Since $\langle Sa, Sb, Sc \rangle$ is also a positive basis, $Sc = -\beta b + \alpha c$ and $S = R(\theta, a)$. \square

We wish to describe the one-parameter subgroups of $SE(3)$.

Exercise 4.8. Let $\xi = \begin{pmatrix} \omega(a) & u \\ 0 & 0 \end{pmatrix} \in \mathfrak{se}(3)$, where $a, u \in \mathbb{R}^3$, $|a| = 1$. Show that

$$\sigma(\theta) := \exp(\theta \xi) = \begin{pmatrix} R(\theta, a) & (I - R(\theta, a))(a \times u) + \langle a, u \rangle a \theta \\ 0 & 1 \end{pmatrix}$$

is the one-parameter subgroup of $SE(n)$ corresponding to ξ .

Proposition 4.4. The exponential map $\exp : \mathfrak{se}(3) \rightarrow SE(3)$ is surjective.

Proof. First note that

$$\exp \left(\begin{pmatrix} 0 & u \\ 0 & 0 \end{pmatrix} \right) = \begin{pmatrix} I & u \\ 0 & 1 \end{pmatrix}.$$

Therefore, we may assume that $A \in SE(3)$ has the form $A = \begin{pmatrix} S & u \\ 0 & 1 \end{pmatrix}$, where $S \in SO(3)$ is not equal to the identity I . We already know that $S = R(\theta, a)$ for some unit vector $a \in \mathbb{R}^3$ and some $\theta \in (0, 2\pi)$. Thus it suffices to show that the transformation $T_a : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ defined by

$$T_a : w \mapsto (I - R(\theta, a))(a \times w) + \langle a, w \rangle a \theta$$

is nonsingular. Let b and c be unit vectors such that $\langle a, b, c \rangle$ form a positive orthonormal basis of \mathbb{R}^3 . Then

$$\begin{aligned} R(\theta, a)a &= a \\ R(\theta, a)b &= b \cos \theta + c \sin \theta \\ R(\theta, a)c &= c \cos \theta - b \sin \theta. \end{aligned}$$

Moreover, for any $S \in SO(3)$, an easy calculation gives $ST_aS^{-1} = T_{Sa}$. Therefore, we may assume without loss of generality that $a = e_1$, $b = e_2$, $c = e_3$. Then

$$\begin{aligned} T_{e_1}e_1 &= \theta e_1 \\ T_{e_1}e_2 &= \sin \theta e_2 + (1 - \cos \theta)e_3 \\ T_{e_1}e_3 &= (-1 + \cos \theta)e_2 + \sin \theta e_3. \end{aligned}$$

The matrix associated to T_{e_1} in the standard basis is

$$\begin{pmatrix} \theta & 0 & 0 \\ 0 & \sin \theta & 1 - \cos \theta \\ 0 & -1 + \cos \theta & \sin \theta \end{pmatrix}.$$

Since the determinant of the above matrix is $2\theta(1 - \cos \theta) \neq 0$, T_{e_1} is nonsingular, concluding the proof. \square

Exercise 4.9. Find the matrix in $SE(3) \subset GL(4, \mathbb{R})$ that corresponds to rotation by $\pi/4$ in the positive direction about the axis that passes through the point $(1, 2, 3)$, parallel to the vector from the origin to the point $(1, 1, 1)$.

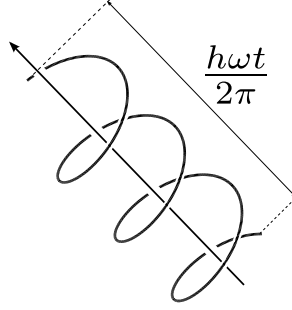


Figure 19: A screw motion in \mathbb{R}^3 consists of a rotation by ωt about an axis l followed by translation parallel to l by $h\omega t/2\pi$, where h is the *pitch* of the screw.

One-parameter subgroups of $SE(3)$ correspond to *screw motions*. A screw S consists of an axis l , a *pitch* h , and a *magnitude* M . A screw motion represents rotation by an angle $M = \omega t$ about the axis l followed by translation by an amount $(h\omega/2\pi)t$ parallel to the axis l . A pure rotation corresponds to $h = 0$ and a pure translation corresponds to $\omega = 0$. Note that, if l is the line through a point p_0 parallel to a vector a , then a screw motion is given by the following rigid transformation:

$$f(p) = p_0 + R(\theta, a)(p - p_0) + \frac{h\theta}{2\pi}a$$

where $\theta = \omega t$. As an element of $GL(4, \mathbb{R})$, f is the matrix

$$\begin{pmatrix} R(\theta, a) & (I - R(\theta, a))p_0 + \frac{h\theta}{2\pi}a \\ 0 & 1 \end{pmatrix}.$$

But we know, from the general form of one-parameter subgroups in $SE(3)$ that

$$(I - R(\theta, a))p_0 + \frac{h\theta}{2\pi}a = I - R(\theta, a)(a \times v) + \langle a, v \rangle a\theta,$$

so $p_0 = a \times v$ and $h = \langle a, v \rangle 2\pi$.

5 MOTION WITH CONSTRAINTS

5.1 KINEMATICS OF LINKED RIGID PARTS

A mechanical system is an ensemble of material parts (or *particles*), with specified mass distribution, and subjected to various kinds of forces. The system is constrained in its motion due to how the parts are linked, the nature of the material, forms of contact between parts,

etc. These constraints can often be represented by specifying a manifold M or, more generally, by subsets of TM when the velocities are also constrained somehow. For example, the set of positions of a pair of rigid balls in \mathbb{R}^3 can be represented by the subset of points (q_1, q_2) in $\mathbb{R}^3 \times \mathbb{R}^3$ such that the distance $|q_2 - q_1|$ is at least the sum of the radii of the two balls. This is a 6 dimensional manifold with boundary. If the balls are linked so as to keep the distance between them constant, the set of configurations reduces to the product $\mathbb{R}^3 \times S^2$, where the first factor gives the position of the center of one ball and S^2 indicates the direction from that center pointing towards the second ball. This space can be written as $SE(3)/H$, where H is the group of symmetries of the two balls system. Certain material properties may be incorporated in our choice of M . For example, just as the motion of a rigid body corresponds to $M = SE(3)$, an elastic but incompressible body might be described in terms of the group $SL(3, \mathbb{R}) \ltimes \mathbb{R}^3$.

In this section we wish to represent the configuration manifold of a system consisting linked rigid parts, in terms of products of elements in the Euclidean group. Thinking of the material body as a graph in which the vertices are the parts and the edges represent links between the parts, we only consider here systems whose graphs are trees. An example of this kind of system is illustrated in Figure 20.

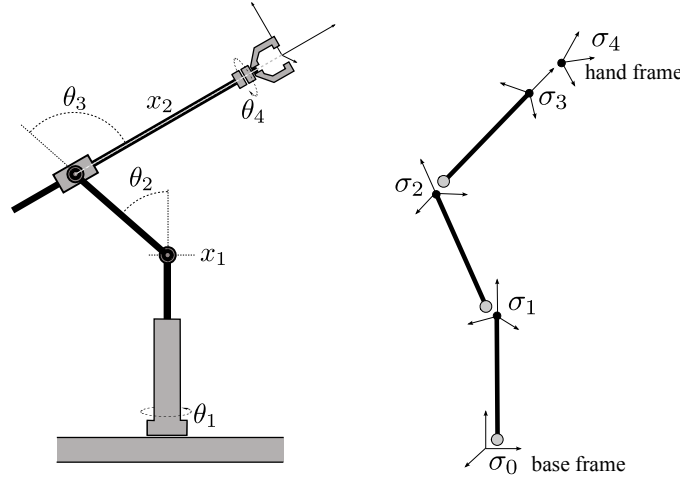


Figure 20: On the left, a schematic robotic arm showing the joint coordinates. On the right, the graph of links. The length of the edges can vary and each affine frame σ_j is rigidly attached to its corresponding part.

We concentrate on the problem of parametrizing the configuration manifold of a system of this kind, ignoring the mass distribution. With this in mind, the structure of links and degrees of freedom at each link can be given a more abstract description in terms of a graph of the type shown in Figure 21.

Each $\sigma_i : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ is an element of $SE(3)$ defining a frame of (affine) Euclidean space which is rigidly attached to the end of the i th arm. If $x = (x_1, x_2, x_3)^t$ is the set of coordinates of a point in space relative to the frame σ_i , then $\sigma_i x$ gives the coordinates of that same point with

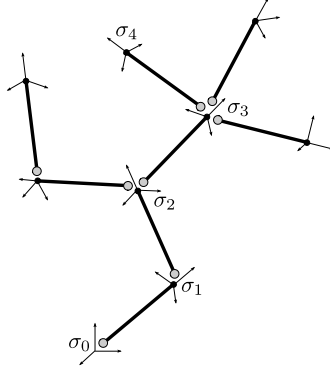


Figure 21: The graph of frames of a system of linked rigid bodies. Two frames linked by an edge are related by $\sigma' = \sigma \circ g$, where σ' is one step farther from the root than σ and g is an element of $SE(3)$. If the graph is a tree then the g are all independent.

respect to the frame σ_0 fixed at the root of the graph (which may be fixed to a work bench, say), taken to be the identity element of $SE(3)$. Let g_i be the element of $SE(3)$ that performs the change of frame from σ_i to σ_{i-1} , where i is the index of an arm directly linked to the arm indexed by $i-1$, so that $\sigma_i = \sigma_{i-1} \circ g_i$. By concatenation of the frame changes along the path of the tree starting at an end finger σ_k to the root σ_0 , we obtain $\sigma_k = g_1 g_2 \dots g_k$. This observation makes it easy to solve the *forward kinematic problem*, that is, the problem of finding the position and orientation of end-effectors given the coordinates representing each σ_i . These coordinates may be regarded as control parameters that can be changed with motors attached to the beginning of each arm. The *backward kinematic problem*, of finding the parameters for a specified position and orientation of the end-effectors is, of course, a much harder problem.

Let us examine the example of Figure 20. The relations between each pair of affine frames is as follows: $\sigma_4 = \sigma_3 \circ g_4(\theta_4)$, $\sigma_3 = \sigma_2 \circ g_3(x_2, \theta_3)$, $\sigma_2 = \sigma_1 \circ g_2(\theta_2)$, $\sigma_1 = \sigma_0 \circ g_1(x_1, \theta_1)$, where the matrices g_j are shown below. The hand frame expressed in terms of the root frame is

$$\sigma_4 = \sigma_0 \circ (g_1(x_1, \theta_1) g_2(\theta_2) g_3(x_2, \theta_3) g_4(\theta_4)) = \sigma_0 \circ g(x_1, x_2, \theta_1, \theta_2, \theta_3, \theta_4).$$

If $x = (x_1, x_2, x_3, 1)^\dagger$ is the coordinate vector of a point in the hand frame, the position of the same point relative to the root frame is then given by $g(x_1, x_2, \theta_1, \theta_2, \theta_3, \theta_4)x$. The matrices g_j are as follows.

$$\begin{aligned}
g_1(x_1, \theta_1) &= \begin{pmatrix} \cos\theta_1 & -\sin\theta_1 & 0 & 0 \\ \sin\theta_1 & \cos\theta_1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & x_1 \\ 0 & 0 & 0 & 1 \end{pmatrix} \\
g_2(\theta_2) &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta_2 & -\sin\theta_2 & 0 \\ 0 & \sin\theta_2 & \cos\theta_2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & l \\ 0 & 0 & 0 & 1 \end{pmatrix} \\
g_3(x_2, \theta_3) &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta_3 & \sin\theta_3 & 0 \\ 0 & -\sin\theta_3 & \cos\theta_3 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & x_2 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \\
g_4(\theta_4) &= \begin{pmatrix} \cos\theta_4 & -\sin\theta_4 & 0 & 0 \\ \sin\theta_4 & \cos\theta_4 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}
\end{aligned}$$

By changing the values of x_i, θ_j independently within their allowed ranges the position of the hand can be controlled.

6 ROLLING AND NON-HOLONOMIC CONSTRAINTS

A typical situation where motion is restricted by conditions on velocities arises in *rolling*. A rigid ball that rolls over a surface without slipping must always be in tangent contact with the surface and the velocity between the point of contact of ball must be zero at all times relative to the point of contact on the surface. We discuss here an example known as the *biplanar bicycle* that nicely illustrates this type of kinematic constraint.

We refer to the system shown in Figure 22. A biplanar bicycle consists of two wheels of radius r that can rotate freely and independently about an axle of length l . A point on each wheel is marked so that we can follow the angle of rotation relative to a horizontal axis perpendicular to the axle. The system configuration is fully specified by giving the angle of each wheel, (θ_0, θ_1) , the position of the center of mass, indicated by its projection (x, y) on the coordinate plane, and the angle ϕ as indicated by the diagram on the right-hand side of Figure 22. These coordinates parametrize the configuration manifold

$$M = \mathbb{T}^2 \times SE(2)$$

where $SE(2)$ is the Euclidian group of motions in dimension 2 and the two-torus is defined here as $\mathbb{T}^2 = \mathbb{R}^2 / (2\pi\mathbb{Z})^2$.

Each point on the wheels is labeled by an element of the disjoint union of two circles $\mathcal{B} = S^1 \cup S^1$. We represent such a point by the pair $(i, [\alpha_i])$, or simply by $[\alpha_i]$, where $i = 0, 1$ (for left, right wheel) and α_i in $[0, 2\pi]$. The reader is asked to check that the position of that point

in \mathbb{R}^3 , given an element $q = ([\theta_0, \theta_1], x, y, [\phi])$ of M and a point $(i, [\alpha_i])$ of \mathcal{B} , is $\Phi : \mathcal{B} \times M \rightarrow \mathbb{R}^3$, where

$$\Phi([\alpha_i], ([\theta_0, \theta_1], x, y, [\phi])) = \begin{pmatrix} x - (-1)^i \frac{l}{2} \sin \phi + r \cos \phi \sin(\alpha_i + \theta_i) \\ y + (-1)^i \frac{l}{2} \cos \phi + r \sin \phi \sin(\alpha_i + \theta_i) \\ r + r \cos(\alpha_i + \theta_i) \end{pmatrix}$$

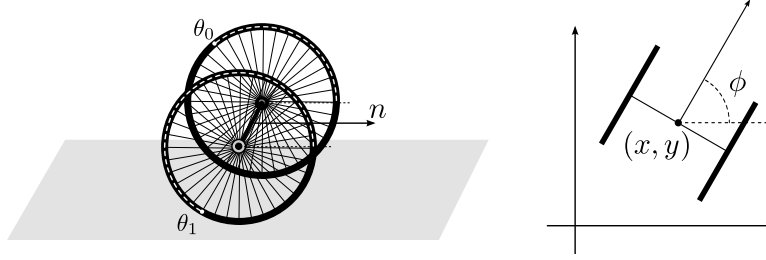


Figure 22:

It will be convenient to write $\Phi_{[\alpha_i]}(q) = \Phi([\alpha_i], q)$. We now suppose that the wheels move without slipping. This imposes a constraint on curves in M specifying the motion of the bicycle. At the contact points of the wheels with the ground, namely, points for which $\alpha_i + \theta_i = \pi$ for $i = 0, 1$ (so that the z -coordinate in \mathbb{R}^3 is 0), the velocity is zero. That is, $(d\Phi_{[\alpha_i]})_q = 0$ if $\alpha_i + \theta_i = \pi$. After an exercise in differentiation, we obtain the constraint equations $\omega_1 = 0, \omega_2 = 0, \omega_3 = 0$ where

$$\begin{aligned} \omega_1 &= dx - r \cos \phi (d\theta_0 + d\theta_1) / 2 \\ \omega_2 &= dy - r \sin \phi (d\theta_0 + d\theta_1) / 2 \\ \omega_3 &= d\phi - r (d\theta_1 - d\theta_0) / l. \end{aligned}$$

The equations $\omega_i = 0$ define a rank 2 subbundle of TM , which is spanned by

$$\begin{aligned} \overline{\frac{\partial}{\partial \theta_0}} &= \frac{r}{2} \left(\cos \phi \frac{\partial}{\partial x} + \sin \phi \frac{\partial}{\partial y} \right) - \frac{r}{l} \frac{\partial}{\partial \phi} + \frac{\partial}{\partial \theta_0} \\ \overline{\frac{\partial}{\partial \theta_1}} &= \frac{r}{2} \left(\cos \phi \frac{\partial}{\partial x} + \sin \phi \frac{\partial}{\partial y} \right) + \frac{r}{l} \frac{\partial}{\partial \phi} + \frac{\partial}{\partial \theta_1} \end{aligned}$$

The Lie bracket of these two vector fields is

$$\left[\overline{\frac{\partial}{\partial \theta_0}}, \overline{\frac{\partial}{\partial \theta_1}} \right] = \frac{r^2}{l} \left(\sin \phi \frac{\partial}{\partial x} - \cos \phi \frac{\partial}{\partial y} \right)$$

This corresponds to infinitesimal motion perpendicular to the wheels of the bicycle. It is the kind of motion one would be used for parallel parking.

6.1 ACCELERATION AND COVARIANT DERIVATIVE

We have already seen how to write the equations of motion associated to a given Lagrangian in coordinates charts by means of the Euler-Lagrange equations. We wish to have a coordinate free way of expressing these equations. But for this we first need to face one key difficulty, having to do with the notion of *acceleration*.

There is no uniquely defined way of defining the acceleration of a smooth path $\gamma : (a, b) \rightarrow M$ when the manifold M is not a vector space. If M is a vector space (or an *affine space* modeled on a vector space) then it makes sense to define the acceleration of γ at a given time t as the limit when h approaches 0 of $(\gamma'(t+h) - \gamma'(t))/h$. But on a general manifold the velocity vectors $\gamma'(t+h)$ and $\gamma'(t)$ live in the different vector spaces $T_{\gamma(t+h)}M$ and $T_{\gamma(t)}M$ and the difference of the velocities does not make sense. What is needed is a well-defined way of transporting a tangent space into another along a curve. Such a notion of transport is provided, in an infinitesimal sense, by the introduction of a *connection*, a term we use interchangeably with *covariant derivative*. On a Riemannian manifold there is a very reasonable choice of connection known as the *Levi-Civita* connection. We will get to it shortly, but in the way of introduction let us first go back to constrained motion in \mathbb{R}^N .

If X is a vector field in \mathbb{R}^N and v is a vector in $T_x\mathbb{R}^N$ for some x , then the derivative of X in the direction v will be denoted by $D_v X$. This is simply the derivative of X along v componentwise. If $X = X_1\partial_1 + \dots + X_N\partial_N$ is the vector field expressed in terms of its component functions, then

$$D_v X = (vX_1)\partial_{x_1} + \dots + (vX_N)\partial_{x_N}.$$

An equivalent, but somewhat more flexible definition is as follows. Let γ be an arbitrary differentiable path representing v (meaning that $\gamma(0) = x$ and $\gamma'(0) = v$.) Then

$$D_v X = \left. \frac{d}{dt} \right|_{t=0} X(\gamma(t)).$$

Yet another characterization of the differentiation of vector fields, D , is as follows. We declare that $D_v X = 0$ for any constant vector field $X = a_1\partial_{x_1} + \dots + a_N\partial_{x_N}$, and that the following properties characterizing a *covariant derivative* hold, where X, X_1, X_2 are differentiable vector fields, f is a differentiable function, and v is a tangent vector:

(c₁) $v \mapsto D_v X$ is a linear map from $T_x\mathbb{R}^N$ to itself;

(c₂) $D_v(X_1 + X_2) = D_v X_1 + D_v X_2$;

(c₃) $D_v(fX) = f(x)D_v X + (vf)X$,

If X is a vector field defined only along a curve $\gamma(t)$ and X is differentiable as a function of the curve parameter, it is still possible to define $D_v X$, where $v = \gamma'(t)$, as follows. Let X_1, \dots, X_N be locally defined vector fields over a region where we wish to differentiate X , and write

$$X(t) = \sum_i f_i(t)X_i(\gamma(t)).$$

Now define

$$\frac{DX}{dt} = \sum_i f'_i(t)X_i(\gamma(t)) + \sum_i f_i(t)D_{\gamma'(t)}X_i.$$

In particular, if $X = \gamma'(t)$ is the velocity vector of a smooth curve γ , its acceleration is naturally defined as

$$\gamma'' = \frac{D\gamma'}{dt}.$$

Although the notation may seem a bit awkward, it will be convenient to be explicit about which covariant derivative is being used; in this case, D is the standard differentiation in \mathbb{R}^N . We will not use the notation γ'' in any other circumstance except for this particular covariant derivative in \mathbb{R}^N . Naturally, 0-acceleration, $D\gamma'/dt = 0$, corresponds to uniform rectilinear motion.

Let now M be a smooth submanifold of \mathbb{R}^N of dimension n . This means that M is a subset of \mathbb{R}^N endowed with a smooth manifold atlas such that the inclusion map is smooth. Typical examples are *hypersurfaces* ($N-1$ -dimensional) submanifolds of \mathbb{R}^N obtained as level sets of regular functions. The sphere of dimension $N-1$, for example, is the level set of the value 1 of the function given by the distance to the origin. Other examples arise in mechanical systems whose material parts are constrained by distance relations among them.

The *normal bundle* $T^\perp M$ is the vector bundle over M whose fibers are

$$T_x^\perp M = \{v \in T_x \mathbb{R}^N : v \cdot u = 0 \text{ for all } u \in T_x M\},$$

where $v \cdot u$ denotes the standard inner product in \mathbb{R}^N . Clearly,

$$T_x \mathbb{R}^N = T_x M \oplus T_x^\perp M.$$

Let Π_x denote for each x the orthogonal projection from $T_x \mathbb{R}^N$ to $T_x M$. If X is a vector field on M locally defined around $x \in M$, and $v \in T_v M$, we set

$$\nabla_v X = \Pi_x D_v X.$$

It can be shown that this vector in $T_x M$ is well-defined, independently of any choice of extension of X to a neighborhood of x in \mathbb{R}^N . (Since, $D_v X = dX(\gamma'(t))/dt|_{t=0}$ for any γ representing v , we can choose γ to lie in M .) Then ∇ is a covariant derivative on TM . An alternative way to define it that does not directly rely on M being a submanifold of Euclidean space will be seen shortly.

If γ is a smooth curve in M and X is a vector field on γ , we define as above the covariant derivative of X along γ by

$$\frac{\nabla X}{dt} = \Pi_{\gamma(t)} \frac{DX}{dt}.$$

When X is the velocity field of γ , then the above represents the tangential component of the curve's acceleration. We say that γ is a *geodesic* on M if

$$\frac{\nabla \gamma'}{dt} = 0.$$

A geodesic on M can then be regarded as the motion of a particle on M that moves freely except for the forces keeping the particle from leaving M . Note that in Exercise 3.2 you have obtained all the geodesics of the n -sphere of radius r in \mathbb{R}^{n+1} .

Exercise 6.1. In addition to the properties (c₁), (c₂), (c₃) characterizing D as a covariant derivative operator, show that D behaves as follows in relation to the standard inner product (dot product) $\langle \cdot, \cdot \rangle$ on \mathbb{R}^N :

$$(c_4) \quad \nu_x \langle X, Y \rangle = \langle D_\nu X, Y \rangle + \langle X, D_\nu Y \rangle$$

$$(c_5) \quad D_X Y - D_Y X = [X, Y]$$

Prove that the above five properties fully characterize D . Also show

$$(c_6) \quad [D_X, D_Y]Z = D_{[X, Y]}Z. \text{ This last property says that } D \text{ is } \textit{flat}. \text{ (More on this and the concept of } \textit{curvature} \text{ later.)}$$

Finally, show that the induced covariant derivative ∇ on vector fields tangent to a submanifold M of \mathbb{R}^N satisfies (c_{*i*}) for $i = 1, 2, 3, 4, 5$, where now $\langle \cdot, \cdot \rangle_q$ is the restriction of dot-product to TM . Show that (c₆) does not hold for spheres.

Definition 6.1 (Levi-Civita connection). Let M be a Riemannian manifold with Riemannian metric $\langle \cdot, \cdot \rangle$. Then a connection ∇ on TM is called the *Levi-Civita* connection of the Riemannian manifold if the above properties (c₄) and (c₅) hold. It will be seen below that these two properties determine a unique connection on TM .

6.2 THE CONNECTION MAP \mathcal{K}

Let us now look at the problem of defining acceleration from a somewhat different viewpoint. First observe that $\eta(t) = \gamma'(t)$ is a path in the manifold $N = TM$. So the second derivative of γ , which is the first derivative of η , is a vector field along η in N , not in M . What is needed then is a map $\mathcal{K}_{\gamma'(t)} : T_{\gamma'(t)}N \rightarrow T_{\gamma(t)}M$ that brings $\gamma''(t)$ back to a tangent vector to M at $\gamma(t)$, but there is no obvious such structure on a smooth manifold structures on M all by itself.

Expressing the problem in more physical terms, note that Newton's second law, which relates the acceleration of a point particle of given mass due to a force acting on the particle, makes an assumption about what is to be regarded as free motion in coordinate 3-space: if there are no forces, then the particle trajectory is such that its velocity is constant, in the sense that the translates of the velocities $v(t_1)$ and $v(t_2)$ at different times t_1, t_2 are equal when translated to a same point. This leads to the concept of an *inertial frame*, which is one in which a particle not subject to any forces does not accelerate. Therefore, acceleration measures deviation from “free” motion when there are forces acting on the particle; and a force is whatever is causing the particle to deviate from free motion as described in an inertial frame. To brake out of this seeming tautology we need to introduce a structure on M that defines what kind of motion should be regarded as unaccelerated. This structure corresponds to a choice of *linear connection*, from which we derive the notion of *parallel translation*.

Now on to the details. The following notation will be used for the differential of a smooth map between manifolds, $f : N \rightarrow M$. If $u \in T_q N$ and $s \mapsto \gamma(s)$ is any smooth path in N representing u , that is, such that $\gamma(0) = q$ and $\gamma'(0) = u$, then the differential of f acting on u is

$$df_q u := \left. \frac{d}{ds} \right|_{s=0} f(\gamma(s)).$$

Then $df_q : T_q N \rightarrow T_{f(q)} M$ is a linear map, which we call the *differential* of f at q .

Definition 6.2 (Connection map). Let M be a smooth manifold and $N = TM$. A family of linear maps $\mathcal{K}_v : T_v N \rightarrow T_q M$, for $v \in N$ and $q = \pi(v)$, is said to be a *connection map* if

1. Whenever ξ is a tangent vector to N at v that can be represented by a path in N of the form $t \mapsto v + tw$, for w also in $T_q M$, then $\mathcal{K}_v \xi = w$. In other words, if $\eta(t)$ is a path in N which is always at the same $T_q M$ for all t , then there is no need to connect tangent spaces, and the ordinary notion of derivative should apply;
2. The correspondence $v \mapsto \mathcal{K}_v$ is *homogeneous* in the following sense: defining $m_c : N \rightarrow N$ by $m_c(v) = cv$, then we require that $\mathcal{K}_{cv} \circ dm_c = c\mathcal{K}_v$;
3. \mathcal{K} is smooth function.

The kernel of $d\pi_v : T_v N \rightarrow T_q M$, where π is the projection $(q, v) \mapsto q$, will be denoted by V_v . It is the n -dimensional subspace of the $2n$ -dimensional space $T_v N$ consisting of those vectors that can be represented by paths of the form $t \mapsto v + tw$, $w \in T_p M$. We call V_v the subspace of $T_v N$ of *vertical* vectors, or the *vertical space* at v . We indicate that ξ is the vertical vector in V_v represented by the path $v + tw \in T_q M$, by writing $\xi = \dot{w}$.

Definition 6.3 (Horizontal subspaces). The kernel of the connection map $\mathcal{K}_v : T_v N \rightarrow T_q M$, for $v \in T_q M$ is called the *horizontal space* at v and denoted H_v . Thus the tangent space of N at each $v \in N$ decomposes as a direct sum $T_v N = H_v \oplus V_v$.

Therefore, if ξ is in the kernel of $d\pi_v$, then $\xi = \dot{w}$ for some $w \in T_p M$ and we require $\mathcal{K}_v \dot{w} = w$ of any connection map \mathcal{K} . In particular, \mathcal{K}_v is surjective and its kernel is the n -dimensional horizontal space H_v .

Definition 6.4 (Acceleration and geodesics). The acceleration, relative to a choice of connection map \mathcal{K} , of a smooth path $\gamma(t)$ in M is the vector in $T_{\gamma(t)} M$ given by $\mathcal{K}_{\gamma'(t)} \gamma''(t)$. The path γ is said to be *geodesic* (relative to \mathcal{K}) if its accelerations is identically 0. In this case $\gamma''(t)$ lies in the horizontal distribution $H_{\gamma'(t)}$ for all t .

An equivalent, and more concrete way of defining a connection on TM is through the notion of a *covariant differentiation*. Let $\eta(t)$ be a differentiable path in TM and $\gamma(t) = \pi(\eta(t))$ the projected path in M . Thus η is a vector field along γ . Define the *covariant derivative* (associated to a connection map \mathcal{K}) of η along γ by

$$\frac{\nabla \eta}{dt}(t) := \mathcal{K}_{\gamma'(t)} \eta'(t).$$

The path $\gamma(t)$ may be singular, say $\gamma'(t) = 0$, even though $\eta'(t)$ may be non-zero. In this case $\eta'(t)$ projects to 0 under the differential of π , so it is a vertical vector, thus $\frac{\nabla \eta}{dt}(t) = \eta'(t)$.

Exercise 6.2 (Basic properties of covariant differentiation). Show that covariant differentiation along a path has the following properties: If $\eta(t), \eta_1(t), \eta_2(t)$ are vector fields along $\gamma(t)$, $f(t)$ is a differentiable function, and a_1, a_2 are real constants, then

1. $\frac{\nabla}{dt}(a_1 \eta_1 + a_2 \eta_2)(t) = a_1 \frac{\nabla \eta_1}{dt}(t) + a_2 \frac{\nabla \eta_2}{dt}(t);$
2. $\frac{\nabla}{dt}(f\eta)(t) = f'(t)\eta(t) + f(t) \frac{\nabla \eta}{dt}(t);$

3. $\frac{\nabla \eta}{dt}(t) = \eta'(t)$ if $\gamma(t)$ is constant in t ;
4. An operation on vector fields along curves satisfying the first three properties arises from a connection map K .
5. If $\eta(t)$ is horizontal, i.e. $\eta(t) \in H_{\gamma(t)}$ for each t , then $\frac{\nabla \eta}{dt} = 0$ and $\gamma(t)$ is a geodesic path.

We say that $t \mapsto \eta(t)$ is a *parallel* vector field along γ if $\frac{\nabla \eta}{dt} = 0$. This equation corresponds in local coordinates a system of linear ordinary differential equations in the vector components of η . A geodesic path is “self-parallel,” that is, $\frac{\nabla \gamma'}{dt} = 0$. We define the covariant derivative of a vector field X on M in the direction $v \in T_q M$ as follows. If γ is a path representing v , then $X(\gamma(t))$ is a path in TM projecting to $\gamma(t)$ under π and

$$\nabla_v X := \left. \frac{\nabla X(\gamma(t))}{dt} \right|_{t=0}$$

at $\gamma(0) = q$. The homogeneity property of \mathcal{K} implies that $\nabla_{cv} X = c \nabla_v X$ and smoothness of \mathcal{K} and X implies that $v \mapsto \nabla_v X$ is smooth. It follows that $v \mapsto \nabla_v X$ is linear in v . Thus we have

Proposition 6.1 (Covariant derivative of vector fields). The connection map \mathcal{K} induces a first order differential operator on vector fields on M satisfying the properties

1. The map $v \mapsto \nabla_v X$ is linear in v ;
2. The map $X \mapsto \nabla_v X$ is linear on the vector space of vector fields on M ;
3. Leibnitz rule: $\nabla_v (fX) = (vf)X + f \nabla_v X$.

Associated to a connection ∇ are two tensor fields on M given in the next definition.

Definition 6.5 (Torsion and curvature tensors). Let X, Y, Z be smooth vector fields on M and ∇ a covariant derivative operator. The *torsion* tensor of ∇ is defined by

$$T(X, Y) := \nabla_X Y - \nabla_Y X - [X, Y]$$

where $[X, Y]$ is the Lie bracket of vector fields. The *curvature* tensor of ∇ is defined by

$$R(X, Y)Z := \nabla_X \nabla_Y Z - \nabla_Y \nabla_X Z - \nabla_{[X, Y]} Z.$$

An operation on vector fields of the form $Z = Q(X_1, \dots, X_k)$, where Z is either a vector field or a function is said to be *tensorial* if it is linear in each argument X_i and for each $q \in M$, $Z(q)$ only depends on the values of the X_i at q . To check that a multilinear function of vector fields is tensorial it suffices to show that

$$Q(X_1, \dots, fX_i, \dots, X_k) = fQ(X_1, \dots, X_i, \dots, X_k)$$

for every smooth function f and each index i . If Q is tensorial, then for each $q \in M$ and vectors $v_i \in T_q M$, the value $z = Q_q(v_1, \dots, v_k)$ is well-defined.

Exercise 6.3 (Tensoriality of T and R). Show that R and T are tensor fields on the manifold M .

Definition 6.6 (Symmetric and flat connections). The connection ∇ is said to be *symmetric* or *torsion-free* if T is identically zero. It is said to be *flat* if R is identically 0.

The significance of the torsion and the curvature tensors becomes clear by observing that these are precisely the obstructions for the manifold to be locally like affine space \mathbb{R}^n . More precisely, the following holds.

Theorem 6.1. If a connection ∇ on TM is flat and torsion-free, then every point of M has a local coordinate neighborhood on which the coordinate vector fields are parallel. In particular, expressed in these local coordinates, geodesics are straight lines with constant velocity, and the manifold is locally isomorphic to \mathbb{R}^n as affine spaces.

Proof. *

□

Suppose now that the manifold M is equipped with a Riemannian metric $g = \langle \cdot, \cdot \rangle$. The metric g is itself a tensor field. If ∇ is a connection on M then it is possible to define the covariant derivative of g (as well as the covariant derivative of any other tensor field, although we do have yet the need for this generality) as follows.

$$(\nabla g)(X, Y, Z) := (\nabla_X g)(Y, Z) := Xg(Y, Z) - g(\nabla_X Y, Z) - g(Y, \nabla_X Z).$$

It is a simply exercise to verify that ∇g is tensorial. When g is a *parallel* tensor in the sense that $\nabla g = 0$, we say that the connection is *metric* (relative to g).

Theorem 6.2 (Levi-Civita connection). On a Riemannian manifold $(M, \langle \cdot, \cdot \rangle)$ there exists exactly one connection ∇ that is both a metric connection and torsion-free. It is called the *Levi-Civita* connection of the Riemannian manifold.

Proof. *

□

We can now return to our Newtonian mechanical systems.

Proposition 6.2 (Newton's second law). Let M be the configuration manifold of a mechanical system and $\langle \cdot, \cdot \rangle$ the kinetic energy Riemannian metric on M . (Recall that the kinetic energy metric is obtained via the position map defined earlier and a choice of mass distribution on the material body.) Suppose that the Lagrangian function of the system has the form

$$L(q, v) = \frac{1}{2} \|v\|_q^2 - U(q)$$

where $U : M \rightarrow \mathbb{R}$ is a smooth potential function. Then the Euler-Lagrange's equations for a motion $\gamma(t)$ can be expressed in terms of the Levi-Civita connection as follows.

$$\frac{\nabla \gamma'}{dt} = -\text{grad}_\gamma U.$$

This is interpreted by saying that the acceleration of γ is proportional to the gradient force associated to the potential function.

Proof. *

□

6.3 ROLLING AND THE CARTAN CONNECTION

7 HAMILTONIAN FORMALISM AND SYMPLECTIC GEOMETRY

It turns out to be very useful to study the equations of motion of a mechanical system on its phase space, or position-velocity space, TM . This is mainly because Newton's second order differential equation on M becomes a first order equation on TM ; but also because the rich geometric structure of the tangent bundle can be used to derive general properties of the system in a particularly elegant and often straightforward way. This is even more so for the cotangent bundle, or position-momentum space T^*M , although we will focus on TM to a greater extent in these notes.

Recall that the Euler-Lagrange equations express the equations of motion of a mechanical system on TM in local coordinates $(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n)$ on the tangent bundle. Our immediate goal is to find a coordinate-free expression of the same equations. The advantages of doing so will, hopefully, become apparent soon. But first, we need to introduce several definitions related to the geometric structure of TM .

7.1 THE LAGRANGIAN ONE-FORM AND ENERGY FUNCTION

We write $N := TM$ for simplicity. The base point projection onto M will be written $\pi : N \rightarrow M$ and $N_q := \pi^{-1}(q) = T_qM$ will denote the vector space fiber above $q \in M$. We often denote elements of N by v , instead of the more explicit (q, v) used earlier, and write $q = \pi(v)$. Being itself a manifold, N has its own tangent bundle $TN = T(TM)$. The kernel V_v of the differential $d\pi_v : T_vN \rightarrow T_qM$ is a vector space of dimension $n = \dim M$, which is canonically isomorphic to T_qM via the linear isomorphism $\mathcal{J}_v : T_qM \rightarrow V_v$ constructed as follows. For each $w \in T_qM$ consider the path $\xi(t) = v + tw$ in N_q . Then $\mathcal{J}_v(w) := \xi'(0)$. It is clear that $\mathcal{J}_v(w)$ projects to 0 under $d\pi_v$, so it belongs to V_v , and that it is injective, hence an isomorphism since V_v and T_qM have the same dimension. In terms of the coordinate vector fields, $\mathcal{J}_v \frac{\partial}{\partial q_j} = \frac{\partial}{\partial \dot{q}_j}$. Let now L be a real valued smooth function on N . The *fiber derivative* of L at $v \in N$ is defined by $\mathbb{F}L_v(w) := dL_v(\mathcal{J}_v(w))$. It will be useful to note that $v \mapsto \mathbb{F}L_v$ is a map from TM to T^*M and that $\mathbb{F}L_v \left(\frac{\partial}{\partial q_j} \right) = \frac{\partial L}{\partial \dot{q}_j}(q, v)$. The quantity $p_j = \frac{\partial L}{\partial \dot{q}_j}$ is called the *momentum* coordinate associated to q_j .

Definition 7.1 (Canonical vector field, Lagrangian 1-form, and energy function). The vector field on N defined by $v \mapsto \mathcal{Z}_v := \mathcal{J}_v(v)$ will be referred to as the *canonical vector field* of TM . Let $L : N \rightarrow \mathbb{R}$ be any smooth function, which we call a *Lagrangian* function on N . The Lagrangian one-form $\Theta = \Theta_L$ associated to L is defined at $v \in N$ by $\Theta_v := dL_v \circ \mathcal{J}_v \circ d\pi_v$. The *energy function* $E = E_L : N \rightarrow \mathbb{R}$ associated to L is defined by $E(v) = \mathcal{Z}L - L$, where $\mathcal{Z}L = dL(\mathcal{Z})$ is the derivative of L in the direction of the canonical vector field.

Let us illustrate these definitions for a Newtonian system on a Riemannian manifold $(M, \langle \cdot, \cdot \rangle)$.

Proposition 7.1 (Lagrangian one-form and energy function for Newtonian systems). Let M be a Riemannian manifold with metric $\langle \cdot, \cdot \rangle$ and Lagrangian $L(v) = \frac{1}{2} \|v\|^2 - U(\pi(v))$. Then the Lagrangian one-form has the form

$$\Theta_v(\xi) = \langle v, d\pi_v \xi \rangle$$

for all $v \in N = TM$ and $\xi \in T_v N$. The energy function for the same system is the sum of the potential and kinetic energies:

$$E(v) = \frac{1}{2} \|v\|^2 + U(\pi(q)).$$

The fiber derivative of L at $v \in N$ is $\mathbb{F}L_v(w) = \langle v, w \rangle$.

Proof. *

□

Exercise 7.1 (Coordinate expressions of E and Θ_L). Let $(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n)$ be a coordinate system on $N = TM$ and $L(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n)$ a smooth function on N . Show that the following hold.

1. The Lagrange one-form Θ is given in coordinates by $\Theta_L = \sum_j \frac{\partial L}{\partial \dot{q}_j} dq_j$.
2. The energy function is $E = \sum_j \dot{q}_j \frac{\partial L}{\partial \dot{q}_j} - L$.
3. Let $\gamma(t)$ be a smooth path in M , so that $\gamma'(t)$ is a smooth path in N . Then $\gamma''(t)$ makes sense as a vector field along the path $t \mapsto \gamma'(t) \in N$. Let $d\Theta$ be the exterior derivative of Θ . Show that

$$\gamma'' \lrcorner d\Theta + dE = \sum_j \left(\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} \right) dq_j$$

where $(u \lrcorner d\Theta)(v) := d\Theta(u, v)$.

4. Let $u_j(t) := q_j(\gamma_j(t))$. Show that

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} = \sum_k \left(\frac{\partial^2 L}{\partial \dot{q}_j \partial \dot{q}_k} u'_k + \frac{\partial^2 L}{\partial \dot{q}_j \partial q_k} u''_k \right) - \frac{\partial L}{\partial q_j}.$$

Proposition 7.2 (Coordinate-free expression of the Euler-Lagrange equations). A smooth path $\gamma : [a, b] \rightarrow M$ is L -critical with fixed endpoints if and only if the path $\eta(t) := \gamma'(t)$ in N is a solution of the differential equation $\eta' \lrcorner d\Theta + dE = 0$.

Proof. This is an immediate consequence of Exercise 7.1.

□

Corollary 7.1 (Conservation of energy). If γ is an L -critical path with fixed endpoints, $E(\gamma'(t))$ is constant in t .

Proof. Taking the derivative in t

$$\frac{d}{dt} E(\gamma'(t)) = dE_{\gamma'(t)}(\gamma''(t)) = -(\gamma''(t) \lrcorner d\Theta)(\gamma'(t)) = -d\Theta(\gamma''(t), \gamma'(t)) = 0.$$

Therefore, $E(\gamma'(t))$ is constant as claimed.

□

We have seen in Proposition 7.2 that for a path $\gamma(t)$ on M to be L -critical it is necessary that γ satisfy the second order differential equation $\gamma'' \lrcorner d\Theta = -dE$. For this to be a regular second-order differential equation, one must be able locally to solve for the second derivative γ'' . Looking at part (4) of Exercise 7.1 we see that in order to solve for γ'' the matrix $(L_{\dot{q}_i \dot{q}_j})$ of second derivatives of L in the velocity coordinates \dot{q}_j must be invertible. If this is the case we say that L is *regular*. For example, if the Lagrangian has the form

$$L(q, v) = \frac{1}{2} Q_q(v) - U(q)$$

where $Q_q(v)$ is a quadratic function in v whose coefficients are functions of q , then by a simple computation we obtain, for a vector $w = (w_1, \dots, w_n)$ in $T_q M$,

$$\sum_{ij} L_{\dot{q}_i \dot{q}_j}(q, v) w_i w_j = Q_q(w).$$

Thus L is regular in this case exactly when Q is a non-degenerate quadratic form. This is always the case for a Newtonian Lagrangian, for which the kinetic energy term is the Riemannian metric of the configuration manifold M .

Exercise 7.2 (Regular Lagrangian). Let L be a smooth real valued function on the n -dimensional manifold M . Show that the following conditions are equivalent.

1. In every coordinate system $(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n)$ of TM the n -by- n matrix $(L_{\dot{q}_i \dot{q}_j}(q, \dot{q}))$ is invertible for all (q, \dot{q}) .
2. In every coordinate system $(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n)$ of TM , the functions on TM

$$q_1, \dots, q_n, \frac{\partial L}{\partial \dot{q}_1}, \dots, \frac{\partial L}{\partial \dot{q}_n}$$

have everywhere linearly independent differentials.

3. In every coordinate system $(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n)$ of TM , defining

$$f_j := q_j, \quad g_j := \frac{\partial L}{\partial \dot{q}_j},$$

then $(f_1, \dots, f_n, g_1, \dots, g_n)$ is also a local coordinate system of TM .

4. The two-form $\omega_L := d\Theta_L$, where Θ_L is the Lagrangian one-form for L , is non-degenerate.
5. The map $\mathbb{F}L: TM \rightarrow T^*M$ is locally invertible.

If L satisfies any of these equivalent conditions, we say that L is *regular*. If $\mathbb{F}L$ is a diffeomorphism from TM to T^*M , then L is said to be *hyperregular*.

Exercise 7.3. We assume here the same notations used in Exercise 7.2, in particular the functions f_j, g_j and the two-form $\omega := \omega_L$. Show that

1. $\Theta = \sum_j g_j dq_j$

2. $\omega = -\sum_j df_j \wedge dg_j$
3. $\xi \lrcorner \omega = \sum_j (dg_j(\xi)df_j - df_j(\xi)dg_j)$ for any $\xi \in TN$
4. $\mathbb{F}L_\nu \frac{\partial}{\partial \dot{q}_j} = g_j(\nu)$
5. Define on T^*M the canonical one-form α such that $\alpha_\eta(X) = \eta(d\pi_\eta X)$, where $\eta \in T^*M$ and π is the base-point map of $T^*M \rightarrow M$. Show that $\mathbb{F}L^* \alpha = \Theta$.

The functions g_j , when the Lagrangian is regular, are called the *momentum* coordinates, although more often one reserves the term for the functions $p_j = g_j \circ (\mathbb{F}L)^{-1}$ defined locally on T^*M . In this case $(q_1, \dots, q_n, p_1, \dots, p_n)$ constitute a system of local coordinates of T^*M . We nevertheless use $p_j := g_j$ in places below and call these functions the *conjugate momentum* coordinates to the q_j .

7.2 THE HAMILTONIAN VECTOR FIELD

Proposition 7.3 (The Hamiltonian vector field). Let Θ and E be the Lagrange one-form and energy function associated to a regular Lagrangian L . In particular, the closed two-form $\omega = d\Theta$ is non-degenerate. Let X be the unique vector field on TM defined by the equation $X \lrcorner \omega = -dE$ and $\pi : TM \rightarrow M$ the base point projection. Then

1. $d\pi_\nu X = \nu$ for all $\nu \in TM$;
2. If a smooth path γ on M is L -critical then the path γ' in TM is an integral curve of X ;
3. If η is an integral curve of X then $\gamma = \pi \circ \eta$ is L -critical.

Proof. *

□

Exercise 7.4 (Hamiltonian vector field in coordinates). Let a given regular Lagrangian be expressed in local coordinates by $L(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_j)$ and let $p_j := \frac{\partial L}{\partial \dot{q}_j}$ be the conjugate momentum coordinates to the q_j . We know that for a regular Lagrangian $(q_1, \dots, q_n, p_1, \dots, p_n)$ also defines a system of local coordinates on $N = TM$. In these new coordinates, write the energy function as $H(q_1, \dots, q_n, p_1, \dots, p_n) = E(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_j)$. Show the following.

1. $\omega = \sum_j dp_j \wedge dq_j$;
2. $X = \sum_j \left(\frac{\partial H}{\partial p_j} \frac{\partial}{\partial q_j} - \frac{\partial H}{\partial q_j} \frac{\partial}{\partial p_j} \right)$;
3. An L -critical path $\gamma(t) = (q_1(t), \dots, q_n(t), p_1(t), \dots, p_j(t))$ satisfies the system of *Hamilton's equations*

$$\dot{q}_j = \frac{\partial H}{\partial p_j}, \quad \dot{p}_j = -\frac{\partial H}{\partial q_j}$$

for $j = 1, \dots, n$.

7.3 LAGRANGIAN SYMMETRIES AND CONSERVATION LAWS

We restrict attention to mechanical systems of the Newtonian type; that is, systems whose configuration manifold is a Riemannian manifold having a Lagrangian function of the form $L(q, v) = \frac{1}{2} \|v\|^2 - U(q)$, where U is the potential function.

Definition 7.2 (Symmetries of the Lagrangian). A *symmetry* of the Newtonian Lagrangian is a smooth diffeomorphism of M that leaves L invariant. More precisely, a diffeomorphism $\varphi : M \rightarrow M$ is a symmetry of L if

$$L(\varphi(q), d\varphi_q v) = L(q, v)$$

for all (q, v) in TM . We say that a complete smooth vector field Y on M is an *infinitesimal symmetry* of L if its flow Φ_t is a one-parameter group of symmetries of L .

Exercise 7.5. Show that a diffeomorphism φ of the Riemannian manifold M is a symmetry of the Newtonian Lagrangian $L(q, v) = \frac{1}{2} \|v\|^2 - U(q)$ if and only if φ is an isometry of M that leaves invariant the potential energy function U .

Proposition 7.4. Let Y be a complete smooth vector field on a Riemannian manifold M with associated flow Φ_s , and L a Newtonian Lagrangian function on $N = TM$ with energy function E and Lagrangian one-form Θ . For any given smooth path $\gamma : [a, b] \rightarrow M$, we define $S(s) := \int_a^b L((\Phi_s \circ \gamma)'(t)) dt$. Then

$$S'(0) = \langle \gamma'(b), Y_{\gamma(b)} \rangle - \langle \gamma'(a), Y_{\gamma(a)} \rangle - \int_a^b \left\langle \frac{\nabla \gamma'}{dt} + \text{grad } U, Y_{\gamma(t)} \right\rangle dt.$$

In particular, if $\gamma(t)$ is an L -critical path and Y is an infinitesimal symmetry of L , then $S'(0) = 0$, the integrand vanishes, and $\langle \gamma'(b), Y_{\gamma(b)} \rangle = \langle \gamma'(a), Y_{\gamma(a)} \rangle$.

Proof. *

□

Corollary 7.2 (Noether's theorem on symmetries and conservation laws). Let a smooth vector field Y on a Riemannian manifold M be an infinitesimal symmetry of the Newtonian Lagrangian $L : TM \rightarrow \mathbb{R}$. Then the quantity $\mathcal{P}_Y(q, v) := \langle v, Y_q \rangle$ is a constant of motion. In other words, if an L -critical path $\gamma(t)$ in M represents the motion of a mechanical system with Lagrangian L , then $t \mapsto \mathcal{P}_Y(\gamma(t), \gamma'(t))$ is constant. We call the function $\mathcal{P}_Y : TM \rightarrow \mathbb{R}$ the *momentum* associated to the infinitesimal symmetry Y .

Proof. This is a corollary of Proposition 7.4.

□

Let us consider one standard example. A Newtonian system of n point masses in \mathbb{R}^3 has the Lagrangian function

$$L(x, v) = \sum_{j=1}^n \frac{1}{2} m_j |v_j|^2 - U(x_1, \dots, x_n)$$

where the potential energy is of the form

$$U(x) = \sum_{i < j} V_{ij}(|x_j - x_i|).$$

The Euclidean group $SE(3)$ acts on the configuration manifold $M = \underbrace{\mathbb{R}^3 \times \cdots \times \mathbb{R}^3}_n$ by

$$g(x_1, \dots, x_n) = (gx_1, \dots, gx_n).$$

Since each g leaves invariant the norm of vectors and the distance between points, it acts by symmetries of the Lagrangian. Now, let $Z = (X, w) \in \mathfrak{se}(3)$ be an element of the Lie algebra of the Euclidean group, where $X \in \mathfrak{so}(3)$ and $w \in \mathbb{R}^3$. We also denote by Z the vector field induced on \mathbb{R}^3 by Z , which has the form $Z_x = Xx + w$, where Xx is interpreted as the matrix multiplication of the skew-symmetric matrix X and the column vector $x \in \mathbb{R}^3$, and w is a column vector in \mathbb{R}^3 . The vector field induced by Z on M is then

$$Z_x = (Xx_1 + w, \dots, Xx_n + w).$$

The momentum function associated to $Z = (X, w) \in \mathfrak{se}(3)$, evaluated at a state (x, v) is then

$$(7.1) \quad \mathcal{P}_Z(x, v) = \sum_{j=1}^n m_j v_j \cdot (Xx_j + w),$$

where we recall that the Riemannian metric on M is given by $\langle v, u \rangle = \frac{1}{2} \sum_{j=1}^n m_j v_j u_j$.

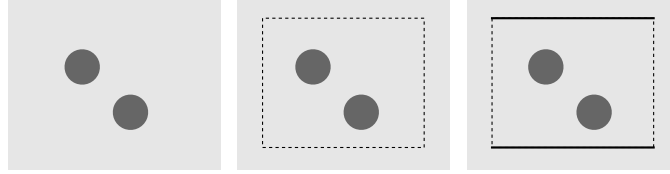


Figure 23: A system of two free discs interacting via elastic collisions. On the left: the ambient space is \mathbb{R}^2 and the symmetry group is $SE(2)$. In the middle: periodic boundary conditions are imposed and the two discs now lie in a torus. In this case the symmetry group reduces to \mathbb{R}^2 acting by translations. On the right, two reflecting, perfectly smooth walls (so that no momentum is exchanged between the walls and the discs tangentially to the walls) are introduced. The motion now is in a cylinder with reflecting circle boundaries. In this case the symmetry group reduces to \mathbb{R} , acting by translations in the horizontal direction. In the first case, linear momentum in the x and y directions and total angular momentum are conserved. In the middle case only the two components of linear momentum are conserved; and in the last case only the x -component of linear momentum is conserved.

The expression 7.1 can be made to look more familiar as follows. We have seen that to each $X \in \mathfrak{so}(3)$ is associated an $a \in \mathbb{R}^3$ such that $Xx = a \times x$. Furthermore, the familiar triple product $v \cdot (a \times x)$ in vector calculus satisfies $v \cdot (a \times x) = -a \cdot (v \times x)$. Therefore, equality 7.1 can be stated as follows. For all $a_j, w \in \mathbb{R}^3$, the quantity

$$\mathcal{P}_Z(x, v) = w \cdot \left(\sum_{j=1}^n m_j v_j \right) - a \cdot \left(\sum_{j=1}^n m_j v_j \times x_j \right)$$

is constant along trajectories of the system. Therefore,

$$P := \sum_{j=1}^n m_j v_j, \quad L := \sum_{j=1}^n m_j x_j \times v_j$$

are, separately, constant. The quantity P is called the *linear momentum*, and L the *angular momentum* of the particle system.

In other cases, the Lagrangian may be invariant under a subgroup of $SE(3)$, rather than the full group. For example, suppose that a pendulum in \mathbb{R}^3 with a rigid rod and pivot fixed at the origin, is subject to a constant acceleration due to gravity. The pivot being fixed reduces the symmetry group to a subgroup of $SO(3)$, and gravity reduces it further to the group $SO(2)$ of rotations about the axis in the direction parallel to the force of gravity through the pivot. Therefore, only the single quantity $e \cdot (v \times x)$ is conserved, where x is the position of the bob, v is its velocity, and e is the direction of gravity.

8 COLLISIONS OF RIGID BODIES

8.1 CONFIGURATION MANIFOLD AND POSITION MAP

We wish to define a system of k rigid bodies in \mathbb{R}^n that are not allowed to overlap. For $j = 1, \dots, k$, let \mathcal{B}_j be a measurable subsets of \mathbb{R}^n and μ_j a finite positive measures on \mathcal{B}_j . We refer to \mathcal{B}_j as a material body with math distribution μ_j and total math $m_j = \mu_j(\mathcal{B}_j)$. It will be convenient to assume that each body has center of mass at 0, that is, we assume

$$\int_{\mathcal{B}_j} b d\mu_j(b) = 0.$$

We denote by \mathcal{B} the disjoint union of the \mathcal{B}_j . Formally, \mathcal{B} may be defined as the subset of $\{1, \dots, k\} \times \bigcup_j \mathcal{B}_j$ consisting of pairs (j, b) such that $b \in \mathcal{B}_j$. We typically omit the index j if there is no possibility of confusion. Let now $G = SE(n)$ be the group of Euclidean motions in \mathbb{R}^n . A system of non-overlapping rigid bodies \mathcal{B}_j has configuration manifold M defined as the closure of the set M_0 that consists of the $(g_1, \dots, g_k) \in G \times \dots \times G$ such that $g_i \mathcal{B}_i$ and $g_j \mathcal{B}_j$ are disjoint for all $i \neq j$. It will be assumed whenever necessary that M is a manifold with corners. Elements of M will be written as $q = (g_1, \dots, g_k)$. Recall that $g_j = (A_j, a_j) \in SO(n) \ltimes \mathbb{R}^n$ and that g_j acts on $b \in \mathcal{B}_j$ by $g_j(b) = A_j b + a_j$. The position map, denoted $\Phi: M \times \mathcal{B} \rightarrow \mathbb{R}^n$, is given by $\Phi(q, (j, b)) = g_j(b)$. When convenient we write $\Phi_q(b) = \Phi(q, (j, b))$.

8.2 THE RIEMANNIAN METRIC

Given $\xi \in \mathfrak{g}$, let ξ^l and ξ^r denote, respectively, the left-invariant and right-invariant vector fields on G associated to ξ . Thus, for each $g \in G$, ξ_g^l and ξ_g^r are the elements of $T_g G$ given by

$$\xi_g^l = (dL_g)_e \xi = \left. \frac{d}{ds} \right|_{s=0} g e^{s\xi}, \quad \xi_g^r = (dR_g)_e \xi = \left. \frac{d}{ds} \right|_{s=0} e^{s\xi} g$$

where L_g and R_g denote left and right-multiplication by g . Regarding \mathfrak{g} as the tangent space to G at e , we have the natural identification $TG \cong G \times \mathfrak{g}$ given by $(g, \xi) \mapsto \xi_g^l$. From this we obtain

the identification $TM = TG \times \cdots \times TG \cong G \times \cdots \times G \times \mathfrak{g} \times \cdots \times \mathfrak{g}$. Each $v \in T_q M$ gives rise to a vector field V_v over \mathcal{B} defined by $V_v(j, b) = (d\Phi_b)_q v$. Note that $V_v(j, b)$ is a tangent vector to \mathbb{R}^n at $g_j(b)$. We will write $V_v(j, b) = V_v(b)$ when the index j is clear in context.

We can now introduce the kinetic energy Riemannian metric on M by defining the inner product of $u, v \in T_q M$ as

$$\langle u, v \rangle_q = \sum_{j=1}^k \int_{\mathcal{B}_j} V_u(b) \cdot V_v(b) d\mu_j(b).$$

It is not difficult to see that this metric is invariant under the left action of G on M given by $g(g_1, \dots, g_k) = (gg_1, \dots, gg_k)$. In fact, writing $g_j = (A_j, a_j)$ and $\xi_j = (Z_j, z_j)$, we have

$$V_v(b) = \frac{d}{ds} \Big|_{s=0} g_j e^{s\xi_j} b = \frac{d}{ds} \Big|_{s=0} \left(A_j e^{sZ_j} b + A_j \int_0^s e^{tZ_j} z_j dt + a_j \right) = A_j (Z_j b + z_j)$$

for each $(j, b) \in \mathcal{B}$ and $v = (v_1, \dots, v_k) = ((\xi_1)_{g_1}^l, \dots, (\xi_k)_{g_k}^l) \in T_q M$. (We have used above the general form of the exponentiation in $SE(n)$ obtained earlier.) Therefore, as A_j leaves invariant the standard inner product in \mathbb{R}^n , we conclude that

$$V_u(b) \cdot V_v(b) = (Z_j^u b + z_j^u) \cdot (Z_j^v b + z_j^v).$$

8.3 MOMENTUM MAP

Let now $U : M \rightarrow \mathbb{R}$ be a potential function. We assume that L is G -invariant, so that the Newtonian Lagrangian

$$L(q, v) = \frac{1}{2} \langle v, v \rangle_q - U(q)$$

is G -invariant. If collisions between the bodies are described (ignoring energy dissipation) by strong (repelling) potential forces of very short range acting between pairs of points, then it is natural to assume that the collision process admits the symmetry group G . This leads to the conservation laws of linear and angular momentum, as we recall now.

Each $\xi \in \mathfrak{g}$ induces a vector field $\tilde{\xi}$ on M whose value at $q = (g_1, \dots, g_k)$ is defined by

$$\tilde{\xi}_q = \frac{d}{ds} \Big|_{s=0} e^{s\xi} q = (\xi_{g_1}^r, \dots, \xi_{g_k}^r).$$

Then the momentum map $\mathcal{P} : TM \rightarrow \mathfrak{g}^*$, where \mathfrak{g}^* is the dual space to \mathfrak{g} , is defined by

$$\mathcal{P}(q, v)(\xi) := \langle v, \tilde{\xi}_q \rangle_q.$$

For $h \in G$ let Ad_h be the linear endomorphism of \mathfrak{g} defined as the differential at identity $e \in G$ of $g \mapsto h^{-1}gh$. Since conjugation by h fixes the identity element, its differential is a linear map from $T_e G = \mathfrak{g}$ to itself.

Proposition 8.1. The momentum map is G -equivariant: $\mathcal{P} \circ g = \text{Ad}_g^* \circ \mathcal{P}$ for all $g \in G$.

Proof. First note that

$$\tilde{\xi}_{gq} = \frac{d}{ds} \Big|_{s=0} e^{s\xi} gq = \frac{d}{ds} \Big|_{s=0} g g^{-1} e^{s\xi} gq = \frac{d}{ds} \Big|_{s=0} g e^{s\text{Ad}_g \xi} q = dg_q(\text{Ad}_g \xi)_q^\sim.$$

Here dg_q is the differential of the left translation operation on G^k by (g, \dots, g) . Therefore,

$$\mathcal{P}(g(q, v))(\xi) = \langle dg_q v, \tilde{\xi}_{gq} \rangle_{gq} = \langle dg_q v, dg_q(\text{Ad}_g \xi)_q^\sim \rangle_{gq} = \langle v, (\text{Ad}_g \xi)_q^\sim \rangle_q = \mathcal{P}(q, v)(\text{Ad}_g(\xi)),$$

proving the claim. \square

Theorem 8.1. Suppose that the Lagrangian function $L : TM \rightarrow \mathbb{R}$ is invariant under the induced action on TM of a Lie group G acting smoothly by diffeomorphisms of M . Then $t \mapsto \mathcal{P}(q(t), v(t))$ is a constant element of \mathfrak{g}^* for any integral curve $t \mapsto (q(t), v(t))$ of the Hamiltonian vector field (on TM).

Proof. * \square

We wish to obtain a more explicit expression for the momentum \mathcal{P} for the case of k rigid bodies. Let $q = (g_1, \dots, g_k)$, $g_j = (A_j, a_j)$, and $v = (v_1, \dots, v_k) \in T_q M$. We choose for each v_j a representative curve of the form $g_j(s) = e^{s\xi_j} g_j$, where $\xi_j = (Z_j, z_j) \in \mathfrak{g}$. For each $(j, b) \in \mathcal{B}$ recall that

$$V_v(j, b) = \frac{d}{ds} \Big|_{s=0} \Phi(g_j(s), b) = \frac{d}{ds} \Big|_{s=0} e^{s\xi_j} g_j b = Z_j A_j b + Z_j a_j + z_j.$$

Here $\Phi(g_j(s), b) = g_j(s)b = A_j(s)b + a_j(s)$ and $A_j(s)b$ is interpreted as matrix product, where b is a column vector. Then for any $\xi = (Z, z) \in \mathfrak{g}$ we obtain that the contribution to $\langle v, \tilde{\xi}_q \rangle_q$ due to body \mathcal{B}_j is

$$\int_{\mathcal{B}_j} V_v(j, b) \cdot V_{\tilde{\xi}_q}(j, b) d\mu_j(b) = \int_{\mathcal{B}_j} [Z_j A_j b + Z_j a_j + z_j] \cdot [Z A_j b + Z a_j + z] d\mu_j(b).$$

Recall that $\int_{\mathcal{B}_j} d\mu_j(b) = m_j$ and $\int_{\mathcal{B}_j} b d\mu_j(b) = 0$. Also note that $x_{cj} := g_j 0 = a_j$ is the center of mass of body \mathcal{B}_j in configuration g_j and that $v_{cj} := V_j(0) = Z_j a_j + z_j$ is the velocity of the center of mass of body \mathcal{B}_j in state (g_j, ξ_j) . Thus we can write

$$(8.1) \quad \langle v, \tilde{\xi}_q \rangle_q = \sum_{j=1}^k \int_{\mathcal{B}_j} (Z_j A_j b) \cdot (Z A_j b) d\mu_j(b) + \sum_{j=1}^k m_j v_{cj} \cdot (Z x_{cj} + z).$$

Before simplifying the above expression further, we need to introduce a few concepts.

Definition 8.1 (Inertia matrix). The inertia matrix of a body $\mathcal{B} \subset \mathbb{R}^n$ with mass distribution measure μ is the n -by- n symmetric matrix L whose (i, j) -entry is given by

$$L_{ij} = \int_{\mathcal{B}} b_i b_j d\mu(b).$$

Exercise 8.1. Let L be the inertia matrix of $\mathcal{B} \subset \mathbb{R}^n$ with mass distribution measure μ . Show the following.

1. For arbitrary n -by- n matrices A_1 and A_2 ,

$$\int_{\mathcal{B}} (A_1 b) \cdot (A_2 b) d\mu(b) = \text{Tr}(A_1 L A_2^\dagger).$$

2. If $g = (A, a) \in SE(n)$, then the inertia matrix of $g\mathcal{B}$ is $L^g := ALA^\dagger$.
3. If \mathcal{B} is a ball centered at $0 \in \mathbb{R}^n$ and μ is invariant under the rotation group $SO(n)$, then L is a multiple of the identity matrix, $L = \lambda I$. Compute the value of λ if the mass distribution of the ball of radius r is uniform.

Definition 8.2. For any two vectors a, b in \mathbb{R}^n we defined $a \wedge b$ to be the skew-symmetric matrix with (i, j) -entry $(a \wedge b)_{ij} = a_i b_j - a_j b_i$. Note that $a \wedge b$ belongs to the Lie algebra $\mathfrak{so}(n)$ of the rotation group $SO(n)$.

Exercise 8.2. Let a, b, u be (column) vectors in \mathbb{R}^n and $Z \in \mathfrak{so}(n)$. Show the following.

1. $(a \wedge b)u = (b \cdot u)a - (a \cdot u)b$.
2. $\text{Tr}((a \wedge b)Z^\dagger) = 2a \cdot (Zb)$.

We now return to the task of simplifying the expression 8.1 for $\mathcal{P}(q, v)(\xi)$. Using the facts stated in Exercise 8.2 we can write

$$\int_{\mathcal{B}_j} (Z_j A_j b) \cdot (Z A_j b) d\mu_j(b) = \text{Tr}(Z_j A_j L_j A_j^\dagger Z^\dagger) = \text{Tr}(Z_j L_j^{g_j} Z^\dagger)$$

and

$$v_{cj} \cdot (Z x_{cj} + z) = \frac{1}{2} \text{Tr}((v_{cj} \wedge x_{cj}) Z^\dagger) + v_{cj} \cdot z.$$

Thus we obtain

$$\langle v, \tilde{\xi}_q \rangle_q = \text{Tr} \left[\left(\sum_{j=1}^k Z_j L_j^{g_j} + \frac{1}{2} v_{cj} \wedge x_{cj} \right) Z^\dagger \right] + \sum_{j=1}^k m_j v_{cj} \cdot z.$$

Exercise 8.3. Let A and Z be n -by- n symmetric and skew-symmetric matrices, respectively, and B an arbitrary n -by- n matrix. Show the following.

1. $\text{Tr}(AZ) = 0$.
2. $\text{Tr}(BZ) = \text{Tr}\left(\frac{B-B^\dagger}{2}Z\right)$.
3. $\text{Tr}(BZ) = 0$ for all skew-symmetric n -by- n matrix Z if and only if B is symmetric.

It is convenient to introduce the operation

$$\mathcal{L}_j^{g_j}(Z_j) := Z_j L_j^{g_j} + L_j^{g_j} Z_j.$$

Note that this is a skew-symmetric matrix. Using the facts from Exercise 8.3 we conclude the following.

Proposition 8.2. Let $q = (g_1, \dots, g_k)$, $g_j = (A_j, a_j)$, and $v = (v_1, \dots, v_k) \in T_q M$. We choose for each v_j a representative curve of the form $g_j(s) = e^{s\xi_j} g_j$, where $\xi_j = (Z_j, z_j) \in \mathfrak{g}$. Then for all $\xi = (Z, z) \in \mathfrak{g}$ the momentum map evaluated at ξ can be written as

$$\mathcal{P}(q, v)(\xi) = \frac{1}{2} \text{Tr} \left[\sum_{j=1}^k \left(\mathcal{L}_j^{g_j}(Z_j) + m_j v_{cj} \wedge x_{cj} \right) Z^\dagger \right] + \sum_{j=1}^k m_j v_{cj} \cdot z.$$

If $(q(t), v(t))$ is a trajectory of a mechanical system having a G -invariant Lagrangian function, then $\mathcal{P}(q(t), v(t))(\xi)$ is constant for all $\xi \in \mathfrak{g}$, from which we conclude that

$$\left(\sum_{j=1}^k \left(\mathcal{L}_j^{g_j}(Z_j) + m_j v_{cj} \wedge x_{cj} \right), \sum_{j=1}^k m_j v_{cj} \right) \in \mathfrak{g}$$

is a constant of motion. The first term of the pair is the total angular momentum of the system, and the second term is the total linear momentum.

Considering the motion of a single body, $k = 1$, we obtain from $\frac{d}{dt} \mathcal{P}(q, v) = 0$ the following. First, $\frac{dv_c}{dt} = 0$ and $\frac{d}{dt}(v_c \wedge x_c) = \frac{dv_c}{dt} \wedge x_c + v_c \wedge v_c = 0$. On the other hand, a straightforward algebraic manipulation gives

$$0 = \frac{d}{dt} \mathcal{L}^g(Z) = \mathcal{L}^g(\dot{Z}) - [\mathcal{L}^g(Z), Z]$$

where \dot{Z} indicates time derivative. Also note that $a = x_c$, $\dot{a} = v_c = Za + z$. Since v_c is constant, $a(t) = v_c(0)t + x_c(0)$ and $z(t) = v_c(0) - Z(t)a(t)$ are determined from the initial conditions and from $Z(t)$, which is the solution to Euler's equation

$$\mathcal{L}^g(\dot{Z}) = [\mathcal{L}^g(Z), Z].$$

For a system of not necessarily free k rigid bodies whose Lagrangian function is G -invariant, we still have the relations:

$$(8.2) \quad \sum_{j=1}^k m_j \dot{v}_{cj} = 0$$

$$(8.3) \quad \sum_{j=1}^k \left(\mathcal{L}_j^{g_j}(\dot{Z}_j) - [\mathcal{L}_j^{g_j}(Z_j), Z_j] + m_j \dot{v}_{cj} \wedge x_{cj} \right) = 0$$

Proposition 8.3. Let $M_n(\mathbb{R})$ denote the space of n -by- n real matrices. For a given $L \in M_n(\mathbb{R})$ define the linear map $\mathcal{L} : M_n(\mathbb{R}) \rightarrow M_n(\mathbb{R})$ by $\mathcal{L}(Z) = ZL + LZ$. Then, if L is symmetric, positive definite, \mathcal{L} is an isomorphism.

Proof. Let $\lambda_1, \dots, \lambda_l$ be the distinct eigenvalues and V_1, \dots, V_l the respective eigenspaces for L . Let $\pi_j : \mathbb{R}^n \rightarrow V_j$ denote the orthogonal projections. Then $\pi_j L = L \pi_j = \lambda_j \pi_j$. It suffices to show that \mathcal{L} has trivial kernel. Thus suppose that $\mathcal{L}(Z) = 0$. Then for all i, j ,

$$0 = \pi_i \mathcal{L}(Z) \pi_j = \pi_i LZ \pi_j + \pi_i ZL \pi_j = (\lambda_i + \lambda_j) \pi_i Z \pi_j.$$

Positivity of the eigenvalues implies that all the blocks $\pi_i Z \pi_j$ are zero. Therefore, $Z = 0$. \square

8.4 COLLISION MAPS AND BOUNDARY CONDITIONS

We now restrict to the case of two bodies, $k = 2$, and wish to describe the outcome of a collision event. So let $q = (g_1, g_2) \in M$ be a collision configuration. We assume that q is a regular point in the boundary of M , in the sense that some open neighborhood of q is diffeomorphic to an open neighborhood of 0 in the upper half-space in $\mathbb{R}^{\dim M}$. We make the further assumptions about the nature of the collision contained in the following definition.

Definition 8.3 (Collision maps). Let $q \in M$ be a regular boundary point in the boundary of M and denote by \mathfrak{n}_q the inward pointing unit normal vector to the boundary of M at q . Define the half-spaces $T_q^+ M = \{v \in T_q M : \langle v, \mathfrak{n}_q \rangle > 0\}$ and $T_q^- M = \{v \in T_q M : \langle v, \mathfrak{n}_q \rangle < 0\}$. We define a *collision map* at q to be an invertible linear map $\mathcal{C}_q : T_q M \rightarrow T_q M$ sending $T_q^- M$ into $T_q^+ M$. In particular, \mathcal{C}_q sends the tangent space to the boundary of M at q to itself. Further assumptions we may impose on \mathcal{C}_q are:

1. *Energy conservation.* \mathcal{C}_q is a linear isometry of the kinetic energy Riemannian metric: $\|\mathcal{C}_q v\| = \|v\|$ for all $v \in T_q M$. Since this implies preservation of the inner product at q and as the tangent space to the boundary of M at q is mapped to itself, energy conservation implies that $\mathcal{C}_q \mathfrak{n}_q = -\mathfrak{n}_q$.
2. *Momentum conservation.* $\langle \mathcal{C}_q v, \tilde{\xi}_q \rangle = \langle v, \tilde{\xi}_q \rangle$ for all $v \in T_q M$ and all $\xi \in \mathfrak{g}$. Recall that $\tilde{\xi}$ is the (right-invariant) vector fields induced on $M = G \times G$ by the natural action of G on the product by left-translations.
3. *Time reversibility.* If $v^+ = \mathcal{C}_q v^-$, then $-v^- = \mathcal{C}_q(-v^+)$, for all $v^- \in T_q^- M$. Because we are assuming that \mathcal{C}_q is linear, this is equivalent to $\mathcal{C}_q^2 = I$.

By a *boundary condition* to the two bodies system we mean a choice of collision map \mathcal{C}_q for each $q \in \partial M$.

Momentum conservation is a consequence of G -invariance of the Lagrangian function, which is physically interpreted by saying that \mathbb{R}^n is physically isotropic and homogenous, and that the Lagrangian function cannot detect an intrinsic position and orientation in space. This also implies that a choice of boundary condition should be G -invariant, that is,

$$dg_q \mathcal{C}_q v = \mathcal{C}_{g(q)} dg_q v$$

for all $g \in G$ and any collision state (q, v) .

It is interesting to note that the conservation laws and time reversibility are not enough in general to specify the map \mathcal{C}_q uniquely. Further assumption on the collision map may be regarded as assumptions about the nature of the contact (slippery, rubbery, etc.) For a description of all the collision maps compatible with the three assumptions of Definition 8.3, it is useful to introduce the linear span $\tilde{\mathfrak{g}}_q \subset T_q M$ of the $\tilde{\xi}_q$ for all $\xi \in \mathfrak{g}$. Since the ∂M is invariant under the action of G , $\tilde{\mathfrak{g}}_q$ is contained in the tangent space to the boundary of M at q . Note that \mathcal{C}_q satisfying the conditions of Definition 8.3 must fix all the vectors in $\tilde{\mathfrak{g}}_q$. In fact, from $\|\tilde{\xi}_q\|^2 = \langle \mathcal{X}_q \tilde{\xi}_q, \tilde{\xi}_q \rangle$, due to conservation of momentum, and $\|\mathcal{C}_q \tilde{\xi}_q\| = \|\tilde{\xi}_q\|$, due to conservation of energy, we conclude that

$$\|\tilde{\xi}_q\|^2 = \langle \mathcal{C}_q \tilde{\xi}_q, \tilde{\xi}_q \rangle = \|\mathcal{C}_q \tilde{\xi}_q\| \|\tilde{\xi}_q\| \cos \theta = \|\tilde{\xi}_q\|^2 \cos \theta$$

where θ is the angle between $\mathcal{C}_q \tilde{\xi}_q$ and $\tilde{\xi}_q$. Therefore, $\cos \theta = 1$ and $\mathcal{C}_q \tilde{\xi}_q = \tilde{\xi}_q$ as claimed.

Proposition 8.4. The set of collision maps satisfying the three conditions of Definition 8.3 is in one-to-one correspondence with the isometric involutions of $W(q) := (\tilde{\mathfrak{g}}_q \oplus \mathbb{R}\mathfrak{n}_q)^\perp \cong \mathbb{R}^m$, where $m = \frac{n^2+n}{2} - 1$. Here n is the dimension of the ambient Euclidean space of the two bodies. The space of linear isometric involutions of \mathbb{R}^m is a disjoint union $\mathcal{J}_0 \cup \dots \cup \mathcal{J}_m$ of the homogeneous spaces $\mathcal{J}_p = O(m)/O(p) \times O(m-p)$, for which $\dim \mathcal{J}_p = p(m-p)$.

Proof. Let C be a linear involution in $O(m)$. Then C is diagonalizable over \mathbb{R} , with eigenspace decomposition

$$\mathbb{R}^m = \left(\frac{C+I}{2} \right) \mathbb{R}^m \oplus \left(\frac{C-I}{2} \right) \mathbb{R}^m$$

and eigenvalues $1, -1$, with respective multiplicities $p, m-p$, where $p \in \{0, 1, \dots, m\}$. Thus for each C there is $p \in \{0, 1, \dots, m\}$ and invertible m -by- m real matrix A such that $C = A^{-1} J_p A$, where $J_p = \text{diag}(I_p, -I_{m-p})$ is the block matrix with diagonal blocks the identity matrices in dimension p and $m-p$. An orthogonal involution is also symmetric, hence we can take A also to be orthogonal. It follows that for each p , C lives in the quotient of $O(m)$ by the isotropy subgroup of J_p under conjugation, which is easily seen to be $O(p) \times O(m-p)$. \square

The following table gives the dimension of \mathcal{J}_p for a few values of n and p .

		p									
		0	1	2	3	4	5	6	7	8	9
$\dim \mathcal{J}_p :$	$n \quad m$										
	1 0	0									
	2 2	0	1	0							
	3 5	0	4	6	6	4	0				
	4 9	0	8	14	18	20	20	18	14	8	0

We see that only in dimension 1 is the outcome of a collision determined only from the conservation laws.

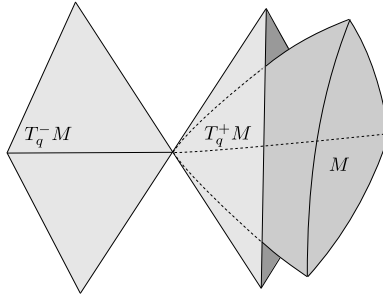


Figure 24: A manifold with corners with the positive and negative cones at a corner point.

Collisions of more than two rigid bodies may often be represented as corner points of a configuration manifold with corners. The general definitions regarding the collision map \mathcal{C}_q

can to some extent apply to this more general situation. Now we interpret $T_q^+ M$ at a corner point to be the cone of inward pointing vectors (see Figure 24) and $T_q^- M = \{-v : v \in T_q^+ M\}$. The conservation laws of energy and momentum, and time reversibility can be stated for $\mathcal{C}_1 : T_q^- M \rightarrow T_q^+ M$ just as for they were stated above for a regular boundary point. When it makes sense to do so, we state results about collisions for any number of bodies, although the case of two bodies is of special interest to us. It is natural to regard collisions of several bodies as consisting of several two bodies collisions happening in close succession.

8.5 IMPULSE VECTORS

At each collision configuration q we define the linear map τ_q on $T_q M$ by $\tau(v) := \mathcal{C}_q v - v$ and call it the *impulse vector*.

Exercise 8.4. Assuming that the collision map \mathcal{C}_q satisfies energy and momentum conservation, and time reversibility, show that the following properties of τ hold.

1. *Conservation of energy.* $\|\tau_q(v)\|^2 = -2\langle \tau_q(v), v \rangle$ for all $v \in T_q M$.
2. *Momentum conservation.* $\tau_q|_{\mathfrak{g}_q} = 0$.
3. *Time reversibility.* $\tau_q^2(v) + 2\tau_q(v) = 0$.
4. τ_q is self-adjoint with eigenvalues 0 and -2 .

At each collision configuration $q = (g_1, \dots, g_q) \in M$ we write $\tau_q = (\tau_1, \dots, \tau_k)$, where τ_j is a linear map from $T_q M$ to $T_{g_j} G$. Let $\xi_j^\tau := (Z_j^\tau, z_j^\tau)$ be the linear map from $T_q M$ into \mathfrak{g} such that $\tau_j = \xi_{g_j}^\tau := \frac{d}{ds}\big|_{s=0} \exp(s\xi_j^\tau) g_j$. Now for each $\xi = (Z, z) \in \mathfrak{g}$ we have

$$\langle \tau_j, \xi_q \rangle_j = \frac{1}{2} \text{Tr} \left[\left(\mathcal{L}_j^{g_j}(Z_j^\tau) + (Z_j^\tau x_{cj} + z_j^\tau) \wedge x_{cj} \right) Z_j^\tau \right] + m_j (Z_j^\tau x_{cj} + z_j^\tau) \cdot z.$$

So for each j the equations $\langle v_j^+ - v_j^-, \xi_q \rangle_j = \langle \tau_j, \xi_q \rangle_j$ for all $\xi \in \mathfrak{g}$ lead to the identities

$$(8.4) \quad \begin{cases} v_{cj}^+ = v_{cj}^- + Z_j^\tau x_{cj} + z_j^\tau \\ Z_j^+ = Z_j^- + Z_j^\tau \\ z_j^+ = z_j^- + z_j^\tau \end{cases}$$

where we have written $v_j^\pm = (\xi_j^\pm)_{g_j}$ and $\xi_j^\pm = (Z_j^\pm, z_j^\pm)$. It was used here that $\mathcal{L}_j^{g_j}$ is invertible. Note that the first of equations 8.4 can be replaced with

$$z^+ = z^- + z^\tau.$$

The conservation laws and time reversibility can be expressed in terms of ξ_j^τ as follows. Momentum conservation gives

$$(8.5) \quad \begin{cases} 0 = \sum_j m_j (Z_j^\tau x_{cj} + z_j^\tau) \\ 0 = \sum_j \mathcal{L}_j^{g_j}(Z_j^\tau) \end{cases}$$

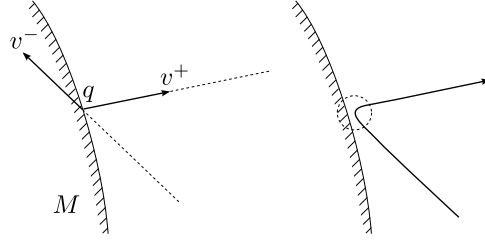


Figure 25: The collision map $v^- \mapsto v^+$ as a limit of strong, short range potential forces acting near the point of contact between the two bodies. The diagram represents the collision process in configuration space M . The tangent vectors v^\pm encode both the velocity of the center of masses and the angular velocities of the two bodies.

We may interpret τ heuristically as follows. We imagine that the colliding bodies interact through strong potential forces that act at very short range around the points of (near) contact. Thus, the two bodies move freely until they come very close to each other, at which moment very strong repelling forces acting on the points of near contact cause the bodies suddenly to move apart and continue on a path of free motion. Let $\gamma(t)$ be a smooth path in configuration space M describing the motion through the entire interaction event. (See the right-hand side of Figure 25, where the process is depicted in the configuration manifold.) We imagine that the interval of time $[t^-, t^+]$ during which the bodies act on each other by non-negligible forces is very short and during this interval the displacements of the two bodies are small, that is, $\gamma(t^-) \approx \gamma(t^+)$, but the derivatives vary nearly discontinuously, so that $v^+ = \gamma'(t^+)$ approximates $\mathcal{C}_q v^-$ where $v^- = \gamma'(t^-)$. Roughly, $\frac{\nabla v}{dt}$ may then be interpreted in the sense of distributions as an infinite force concentrated at a single time t whose time integral is $\tau(v^-)$. We have not yet restricted \mathcal{C}_q in any way. To understand the additional assumption we are about to make first recall that for every $X \in T_q M$, $q = (g_1, g_2)$,

$$\langle \tau, X \rangle = \int_{B_1} V_\tau(b) \cdot V_X(b) d\mu_1(b) + \int_{B_2} V_\tau(b) \cdot V_X(b) d\mu_2(b)$$

where $V_\tau(b)$ may be interpreted as the integral of the distributional force applied to the material point b in configuration g_j . We now assume that this force has a distributional nature relative to integration with respect to μ_j , and that it is concentrated on the point of contact, which we denote by Q . Introducing the notation $\mathcal{J}_j := V_\tau(g_j^{-1}Q)$, we then have

$$\langle \tau, X \rangle = \mathcal{J}_1 \cdot V_X(g_1^{-1}Q) + \mathcal{J}_2 \cdot V_X(g_2^{-1}Q).$$

Note that \mathcal{J}_j is a linear map from $T_q M$ into \mathbb{R}^n . If $X = \tilde{\xi}_q$, $\xi = (Z, z)$ and $V_{\tilde{\xi}_q}(g_j^{-1}Q) = ZQ + z$. So

$$\mathcal{J}_j \cdot V_{\tilde{\xi}_q}(g_j^{-1}Q) = \mathcal{J}_j \cdot (ZQ + z) = \frac{1}{2} \text{Tr}[(\mathcal{J}_j \wedge Q) Z^\dagger] + \mathcal{J}_j \cdot z.$$

From this we obtain

$$\begin{aligned} m_j(Z_j^{\tau}(v^-)x_{cj} + z_j^{\tau}(v^-)) &= \mathcal{I}_j \\ \mathcal{L}_j^{g_j}(Z_j^{\tau}(v^-)) &= \mathcal{I}_j \wedge (Q - x_{cj}) \end{aligned}$$

while equations 8.4 now take the form

$$(8.6) \quad m_j v_{cj}^+ = m_j v_{cj}^- + \mathcal{I}_j$$

$$(8.7) \quad \mathcal{L}_j^{g_j}(Z_j^+) = \mathcal{L}_j^{g_j}(Z_j^-) + \mathcal{I}_j \wedge (Q - x_{cj})$$

with the condition that $\sum_j \mathcal{I}_j = 0$.

9 THE SYMPLECTIC FORM AND SASAKI METRIC ON TM

Let M be a Riemannian manifold with metric $\langle \cdot, \cdot \rangle$. Let ∇ be the Levi-Civita connection and \mathcal{K} the connection map on the tangent bundle of $N = TM$. Recall that \mathcal{K} and ∇ are related as follows. For $v \in N$ and $\xi \in T_v N$, let $v(t)$ be a path in N representing ξ ; that is, $v(0) = v$ and $v'(0) = \xi$. Then

$$\mathcal{K}_v \xi := \left. \frac{\nabla}{dt} \right|_{t=0} v(t).$$

We can similarly express the connection map in terms of the covariant derivative of vector fields as follows. Let Y be a smooth vector field defined on a neighborhood of a point q in M such that $Y(q) = v$. Let w be any vector in $T_q M$. Then $\xi := dY_q w$ is a vector in $T_v N$ projecting to w under the differential of the base-point map $\pi : N \rightarrow M$ (due to the chain rule and the fact that $\pi \circ Y$ is the identity map on M) and

$$\mathcal{K}_v \xi = \nabla_w Y.$$

Also recall that TN splits as a direct sum of subbundles $TN = H \oplus V$ where, at each $v \in N$, the horizontal subspace H_v is the kernel of $\mathcal{K}_v : T_v N \rightarrow T_q M$, $q = \pi(v)$, and V_v is the vertical subspace, defined as the kernel of $d\pi_v : T_v N \rightarrow T_q M$. The projection $d\pi_v$ restricted to H_v is a linear isomorphism onto $T_q M$ and recall that the map $\mathcal{I}_v : T_q M \rightarrow V_v$ is a linear isomorphism such that $\mathcal{K}_v \circ \mathcal{I}_v w = w$ for all $w \in T_q M$.

Proposition 9.1. Let L be the Lagrangian function on N associated to a Newtonian system with a given potential function U on the Riemannian manifold M . Therefore, $L(q, v) = \frac{1}{2} \|v\|^2 - U(q)$. Let $\Theta = \Theta_L$ be the associated Lagrangian one-form. Then

$$d\Theta(\xi_1, \xi_2) = \langle \mathcal{K}_v \xi_1, d\pi_v \xi_2 \rangle - \langle \mathcal{K}_v \xi_2, d\pi_v \xi_1 \rangle$$

for all $v \in N$ and $\xi_1, \xi_2 \in T_v N$.

Proof. *

□

Definition 9.1 (Sasaki metric). The *Sasaki metric* on N is the Riemannian metric on N defined on tangent vectors $\xi_1, \xi_2 \in T_v N$ by

$$\langle \xi_1, \xi_2 \rangle_v := \langle d\pi_v \xi_1, d\pi_v \xi_2 \rangle_q + \langle \mathcal{K}_v \xi_1, \mathcal{K}_v \xi_2 \rangle_q.$$

In other words, the Sasaki metric is characterized by the requirements that H and V be orthogonal subbundles of TN , that the projection $d\pi_v$ be an isometric isomorphism between H_v and $T_q M$, and that \mathcal{K}_v be an isometric isomorphism between V_v and $T_q M$.

It is interesting to note that the symplectic form $\omega = d\Theta$ and the Sasaki metric $\langle \cdot, \cdot \rangle$ are related by $\omega(\cdot, \cdot) = \langle J \cdot, \cdot \rangle$, where $v \mapsto J_v$ is a field of linear isomorphisms on $T_v N$ such that $J_v^2 = -I$ for each v . This means that N has a natural quasi-complex structure. When ∇ is flat, it can be shown that the quasi-complex structure is integrable and N is a complex manifold.

Definition 9.2 (Vertical and horizontal lifts of vector fields). Let Y be a vector field on M . We denote by Y^H the unique vector field on N such that $Y_v^H \in H_v$ and $d\pi_v Y_v^H = Y_q$, $q = \pi(v)$; and by Y^V the unique vector field on N such that $Y_v^V = \mathcal{J}_v Y_q$.

Definition 9.3 (Gradient of a function). Let f be a smooth function on a Riemannian manifold M with Riemannian metric $\langle \cdot, \cdot \rangle$. The *gradient vector field* of f is the vector field on M uniquely determined by the equation $\langle \text{grad}_q f, u \rangle = df_q(u)$.

Proposition 9.2. Let X be the Hamiltonian vector field in N associated to a Newtonian Lagrangian function L with potential energy function U . Let E be the energy function derived from L , X_0 the Hamiltonian vector field on the same space associated to free motion (that is, $U = 0$), which is called the *geodesic spray* of the Riemannian metric on M . Finally, let \mathcal{Z} be canonical vector field on N . The gradient vector field of a function on N is taken with respect to the Sasaki metric. Then $X = X_0 - (\text{grad } U)^V$, $\text{grad } E = \mathcal{Z} + (\text{grad } U)^H$ and $\text{grad } L = \mathcal{Z} - (\text{grad } U)^H$.

Proof. First note that $X - X_0$ is a vertical vector field since both X and X_0 project under $d\pi_v$ to v . Since X_0 is horizontal, $(X - X_0)_v = \mathcal{K}_v X_v$. But this last expression is the acceleration vector, at time $t = 0$, of a solution path to Newton's equation with initial condition (q, v) . Therefore, it is equal to $-\text{grad}_q U$. This shows the first identity. For the second identity first observe that

$$dE_v(\xi) = \omega_v(\xi, X) = \langle \mathcal{K}_v \xi, d\pi_v X \rangle - \langle \mathcal{K}_v X, d\pi_v \xi \rangle = \langle \xi, \mathcal{Z}_v \rangle + \langle \xi, (\text{grad } U)^H \rangle.$$

The second identity follows from this. An easy calculation shows that the gradient of the kinetic energy function $K(q, v) := \frac{1}{2} \|v\|_q^2$ is \mathcal{Z} . The third identity is then a consequence of $E + L = 2K$. \square

A consequence of the proposition is that

$$\|\text{grad}_v E\|_v^2 = \|\text{grad}_v L\|_v^2 = \|v\|_q^2 + \|\text{grad}_q U\|_1^2.$$

As the energy function E is invariant under the Hamiltonian flow, level sets of E are invariant sets. When \mathcal{E} is a regular value of E , the equation $E = \mathcal{E}$ defines a smooth manifold, possibly with boundary, of dimension $2n - 1$, where n is the dimension of M . This is a consequence of the implicit function theorem. The vector field

$$\eta := \text{grad } E / \|\text{grad } E\|$$

is a unit normal vector field to the level sets $N(\mathcal{E})$. The tangent bundle to $N(\mathcal{E})$ is the kernel of the one-form dE ; equivalently, the orthogonal space to η . It follows that

$$T_v N(\mathcal{E}) = \{\xi \in T_v N : d(U \circ \pi)_v \xi + \langle v, \mathcal{K}_v \xi \rangle = 0\}.$$

The restriction of π to $N(\mathcal{E})$ is a *submersion*, that is, $d\pi_v$ maps each tangent space $T_v N(\mathcal{E})$ onto $T_q M$, $q = \pi(v)$. In fact, let $w \in T_q M$ and denote by \bar{w} the horizontal lift of w to v and define

$$\xi = \bar{w} - \frac{dU_q(w)}{\|v\|^2} Z_v.$$

Then $d\pi_v \xi = w$ and

$$d(U \circ \pi)_v \xi + \langle v, \mathcal{K}_v \xi \rangle_q = dU_q(w) + \langle v, -\|v\|_q^{-2} dU_q(w) v \rangle_q = 0$$

Let now S be a smooth hypersurface, or codimension one submanifold, of M . We denote $N_S = \{(q, v) \in N : q \in S\}$ and define $N_S(\mathcal{E}) := N_S \cap N(\mathcal{E})$. Note that for q to be the base point of a state in $N_S(\mathcal{E})$ it is necessary that $\mathcal{E} \geq U(q)$.

Proposition 9.3. Let \mathcal{E} be a regular value of E and S a smooth hypersurface of M , which may be an open subset of regular points of the boundary of M . Then $\xi \in T_v N_S(\mathcal{E})$ if and only if

$$d(U \circ \pi)_v \xi + \langle v, \mathcal{K}_v \xi \rangle = 0$$

and $d\pi_v \xi$ is tangent to S at $\pi(v)$. In particular, the subspaces

$$\{\xi \in V_v : \langle \mathcal{Z}, \xi \rangle_v = 0\} \text{ and } \{\xi \in H_v \cap \ker d(U \circ \pi)_v : d\pi_v \xi \in T_q S\}$$

lie in $T_v N_S(\mathcal{E})$.

Proof. *

□

Proposition 9.4. Let $\omega = d\Theta$ be the symplectic form on $N = TM$. Let i be the inclusion map of $N_S(\mathcal{E})$ into N and define $\omega_S^\mathcal{E} := i^* \omega$. Then $\omega_S^\mathcal{E}$ is a symplectic form on $N_S(\mathcal{E}) \setminus TS$.

Proof. The form $\omega_S^\mathcal{E}$ is the restriction of ω to vectors tangent to $N_S(\mathcal{E})$. There will be little risk of confusion in denoting it simply by ω . This form is closed since d commutes with i^* , so we only need to show that it is also non-degenerate. Let ξ be a vector in $T_v N_S(\mathcal{E})$ and assume that $\omega(\xi, \zeta) = 0$ for all $\zeta \in T_v N_S(\mathcal{E})$ and $v \notin TS$. We first assume that ζ is vertical, so $\langle v, \mathcal{K}_v \zeta \rangle = 0$ by Proposition 8.7 and $\omega(\xi, \zeta) = -\langle d\pi_v \xi, \mathcal{K}_v \zeta \rangle = 0$, where we use the form of ω given by Proposition 8.5. This means that $\langle w, d\pi_v \xi \rangle = 0$ for all $w \perp v$, hence $d\pi_v \xi = \lambda v$ for some real number λ . Since also $d\pi_v \xi \in T_q S$ by Proposition 8.7 and $v \notin T_q S$, we conclude that $d\pi_v \xi = 0$ and ξ is a vertical vector. Therefore, $0 = \omega(\xi, \zeta) = \langle \mathcal{K}_v \xi, d\pi_v \zeta \rangle$ for all $\eta \in T_v N_S(\mathcal{E})$. Because the restriction of $d\pi_v$ to $T_v N_S(\mathcal{E})$ maps onto $T_q S$ as noted in the comments preceding Proposition 8.7, we have $\langle \mathcal{K}_v \xi, w \rangle = 0$ for all $w \in T_q S$. So we have $\mathcal{K}_v \xi = \lambda n_q$, $\lambda \in \mathbb{R}$, where n_q is a unit vector perpendicular to S at q , and $d\pi_v \xi = 0$. Once again by Proposition 8.7, $0 = \langle v, \mathcal{K}_v \xi \rangle = \lambda \langle v, n_q \rangle$. Therefore, $\lambda = 0$ as $\langle v, n_q \rangle \neq 0$, and $\xi = 0$. □

Corollary 9.1. Let S be a smooth hypersurface in the n -dimensional configuration manifold M . Let $N_S(\mathcal{E})$, as defined above, be the set of (q, v) in an energy level set $N(\mathcal{E})$, for a regular value \mathcal{E} , such that $q \in S$. Then $N_S(\mathcal{E})$ is a symplectic manifold of dimension $2n - 2$ with symplectic form given by restriction to $N_S(\mathcal{E})$ of $d\Theta$. The hypersurface may be a smooth open subset of the boundary of M .

The next exercise shows the various concepts introduced in this section in the special case in which M is submanifold of dimension n of \mathbb{R}^n with smooth boundary and Riemannian metric given by the standard inner product in \mathbb{R}^n , denoted by $\langle u, v \rangle = u \cdot v$. Then $N := TM \cong M \times \mathbb{R}^n$ and each element of TN may be written as (q, v, \dot{q}, \dot{v}) , which decomposes as a sum of a horizontal component $(q, v, \dot{q}, 0) \in H_{(q,v)}$ and a vertical component $(q, v, 0, \dot{v}) \in V_{(q,v)}$.

Exercise 9.1. Let $M = \mathbb{R}^n$ with Lagrangian $L(q, v) = \frac{1}{2}|v|^2$, where $|v|^2 = v \cdot v$. Show the following.

1. The Hamiltonian vector field is $X = (q, v, v, 0)$.
2. The Lagrangian one-form is $\Theta = \sum_{j=1}^n v_j dq_j$.
3. The symplectic form is $\omega = \sum_{j=1}^n dv_j \wedge dq_j$.
4. The Sasaki metric on $T\mathbb{R}^n$ is $\sum_{j=1}^n (dq_j \otimes dq_j + dv_j \otimes dv_j)$.
5. The gradient vector field of the energy function is $\text{grad}_{(q,v)} E = (q, v, 0, v)$.
6. The unit normal vector field to the level sets of E is $\eta_{(q,v)} := \frac{\text{grad}_{(q,v)} E}{|\text{grad}_{(q,v)} E|} = \left(q, v, 0, \frac{v}{|v|} \right)$.

10 INVARIANT MEASURES

An essential fact concerning the dynamics of conservative mechanical systems is the existence of volume measures on the phase space, and on level sets of the energy function, that are invariant under the Hamiltonian flow. When the volume of an energy level set is finite one obtains by normalization a natural notion of invariant probability measure. In this section we wish to describe such invariant measures as well as associated invariant measures on the boundary of the phase space energy level sets. In the next section, on ergodic theory, we will derive a number of dynamical conclusions from the existence of these measure.

We consider Newtonian systems on general Riemannian manifolds. Thus let M be an n -dimensional Riemannian manifold, which we allow to have non-empty boundary. The boundary will be denoted S . We assume that the S is a smooth manifold of dimension $n - 1$, although later we may relax this smoothness assumption and consider piecewise smooth boundaries more generally. The Lagrangian is then $L(q, v) = \frac{1}{2}\|v\|^2 - U(q)$ for a smooth potential function U . In systems of billiard type we let $U = 0$. The phase space is $N = TM$, also a manifold with boundary. The energy function and Lagrangian 1-form are denoted, respectively, E and Θ , and the symplectic form ω . The Hamiltonian vector field will be denoted X and the the Hamiltonian flow, which is well-defined in the interior of N , will be denoted Φ_t .

It is necessary to specify how trajectories are to be extended past a time of collision with the boundary. Equivalently, we need to specify how a solution $\gamma(t)$ to Newton's equation

$\frac{\nabla \gamma'}{dt} = -\text{grad } U$ (a path in M) should be defined after it reaches a boundary point. There are different, physically meaningful, choices for boundary condition, but in these notes we will only consider the following one.

Assumption 1 (Boundary condition). When a solution path of Newton's equation reaches a point q in the boundary S of M , its velocity v^+ immediately after collision will be taken to be the specular reflection of the velocity v^- just prior to collision on the tangent plane to the boundary at q .

Let us take a moment to reflect on the physical meaning of this assumption. Consider two convex rigid bodies, \mathcal{B}_1 and \mathcal{B}_2 in \mathbb{R}^3 moving freely in space, and colliding with each other at a given moment. The configuration manifold consists of a subset M of $G_1 \times G_2$, where $G_i = SE(3)$ is the group of Euclidean motions of body \mathcal{B}_i . If the bodies have smooth boundary and are convex, M is a manifold of dimension 12 having a boundary S , which is a smooth manifold of dimension 11. A boundary point of M corresponds to a collision configuration. A tangent vector at a boundary point describes a pre-collision velocity if it points outward (away from M), or a post-collision velocity if it points inward. Vectors $T_q S$ represent grazing motion. If we assume that the boundary surfaces of the the bodies are perfectly polished and physically smooth (rather than, say, rubbery) and that the bodies do not offer any resistance to motion in this tangential direction, then the post-collision velocities of the bodies, represented by the vectors $v^\pm \in T_q M$, are determined as follows. If the map $R : v^- \mapsto v^+$ is linear, which we assume to be the case, then by conservation of energy R must be an isometric isomorphism of $T_q M$. (Recall that the Riemannian metric on M is derived from the kinetic energy.) In particular, $\|v^-\| = \|v^+\|$. The decomposition of a vector $v \in T_q M$ as a sum of a component in $T_q S$ and a component in the direction perpendicular to $T_q S$ corresponds to the decomposition of the state of the system at the moment of collision into a grazing motion and a frontal collision motion. The tangential components of the vectors v^+ and v^- are the same, due to the assumption of physical smoothness. Their components in the direction perpendicular to the boundary must switch signs because v^- points out of M and v^+ points into M . Therefore, R must be a reflection map. Note that other choices for the collision map at boundary points compatible with conservation of linear momentum, angular momentum, energy, and time reversibility are possible. We nevertheless restrict attention here to specular reflections only.

With Assumption 1, we have a well-defined way of extending trajectories for times $t > t_c$ for any collision time t_c . In this way, at least in cases when the potential function U is zero (but in many other cases as well), we have that trajectories are defined for all time. (We will not be concerned with collisions at corners and other singular events, which will typically have probability 0.)

10.1 THE LIOUVILLE MEASURE

We begin by summarizing a few general facts and the notation we will use in this section. We restrict attention to Newtonian systems, for which the Lagrangian function is given by kinetic energy minus potential energy.

- M is the configuration manifold with the kinetic energy Riemannian metric $\langle \cdot, \cdot \rangle$. The

base-point projection map is $\pi : N := TM \rightarrow M$. The Lagrangian function is

$$L(q, v) = \frac{1}{2} \|v\|_q^2 - U(q)$$

where U is a potential function on M . The associated energy function is given by $E(q, v) = \frac{1}{2} \|v\|_q^2 + U(q)$. The Lagrangian one-form is Θ which, for Newtonian systems, is given by

$$\Theta(\xi) = \langle v, d\pi_v \xi \rangle_q.$$

The symplectic form on N is denoted by $\omega := d\Theta$.

- For each $(q, v) \in N$, the vertical lift is the previously defined isomorphism \mathcal{J}_v from $T_q M$ to the vertical subspace $V_v \subset T_v N$. The connection map \mathcal{K}_v goes from $T_v N$ to $T_q M$, $\mathcal{K}_v \circ \mathcal{J}_v$ is the identity map on $T_q M$, and the kernel of \mathcal{K}_v is the horizontal subspace $H_v \subset T_v N$. The symplectic form can be expressed in terms of the connection map and the Riemannian inner product as

$$\omega(\xi_1, \xi_2) = \langle \mathcal{K}_v \xi_1, d\pi_v \xi_2 \rangle - \langle \mathcal{K}_v \xi_2, d\pi_v \xi_1 \rangle$$

for all $v \in N$ and $\xi_1, \xi_2 \in T_v N$. The Sasaki metric is the Riemannian metric on N defined on tangent vectors $\xi_1, \xi_2 \in T_v N$ by

$$\langle \xi_1, \xi_2 \rangle_v := \langle d\pi_v \xi_1, d\pi_v \xi_2 \rangle_q + \langle \mathcal{K}_v \xi_1, \mathcal{K}_v \xi_2 \rangle_q.$$

- The Hamiltonian vector field on N is X , defined by $i_X \omega = -dE$. The energy function is invariant under the Hamiltonian flow. In fact,

$$XE = i_X dE = -\omega(X, X) = 0.$$

We have $d\pi_v X = v$. In fact, let $q = \pi(v)$ and $w \in T_q M$ be arbitrary. Define $\xi := \mathcal{J}_v w$. Then, from the expression of ω given above in terms of the Riemannian metric on M ,

$$i_X \omega(\xi) = -\langle \mathcal{K}_v \xi, d\pi_v X \rangle = -\langle w, d\pi_v X \rangle$$

and it is a simple check to verify that $-dE(\xi) = \langle v, w \rangle$, which we obtain by recalling that $\mathcal{J}_v w$ is represented by the curve in N given by $\xi(t) = v + tw$. We also have

$$\mathcal{K}_v X = -\mathcal{J}_v \text{grad}_q U.$$

This is essentially Newton's equation of motion. It follows that $X = \mathcal{Z} - (\text{grad } U)^V$, where \mathcal{Z} is the canonical vector field and the superscript V denotes vertical lift.

- \mathcal{L}_Z , for a vector field Z , denotes the Lie derivative along Z . Recall that the Lie derivative applied to a differential form α satisfies $\mathcal{L}_Z \alpha = di_Z \alpha + i_Z d\alpha$. The Lie derivative of θ and ω along the Hamiltonian vector field X are $\mathcal{L}_X \theta = dL$ and $\mathcal{L}_X \omega = 0$. The first identity is a consequence of $i_X d\theta = -dE$ and of

$$(i_X \theta)_v = \langle v, d\pi_v X \rangle_q = \|v\|_q^2 = E(q, v) + L(q, v),$$

from which we obtain $di_X \theta = dE + dL$. The second identity now results from $d\mathcal{L}_X = \mathcal{L}_X d$.

Proposition 10.1. Let the dimension of M be n . For Newtonian systems $\Omega := \frac{1}{n!} \omega \wedge \dots \wedge \omega = \frac{1}{n!} \omega^n$ is nowhere vanishing and invariant under the Hamiltonian flow.

Proof. That Ω is nowhere vanishing is due to the Newtonian Lagrangian being regular. Invariance follows from $\mathcal{L}_X \omega = 0$ and since the Lie derivative is an algebraic derivation with respect to the wedge product. \square

Definition 10.1 (Liouville measure). The measure obtained by integration with respect to Ω is called the *Liouville measure*. We will at times denote it by $|\Omega|$. In canonical coordinates,

$$|\Omega| = dq_1 \dots dq_n dp_1 \dots dp_n.$$

Invariance of the energy function E under the Hamiltonian flow means that the Hamiltonian vector field X is tangent to the level sets of E . Let us fix a value \mathcal{E} of E and denote by $N(\mathcal{E})$ the level set for \mathcal{E} . We assume that \mathcal{E} is a regular value so that $N(\mathcal{E})$ is a smooth submanifold of N , possibly with boundary. The boundary of $N(\mathcal{E})$ consists of the ν that project under π to a boundary point of M . We have introduced before the unit normal vector $\eta := \text{grad } E / \|\text{grad } E\|$ to the level sets of E .

Proposition 10.2. Let X be the Hamiltonian vector field for the energy function E , and η the unit normal vector to the level sets of E defined above. Let $\Omega = \frac{1}{n!} \omega^n$ be the invariant volume form on N and define $\Omega_E := i_\eta \Omega$. Then the following hold.

1. $\Omega = dE \wedge \Omega_E$;
2. $i_X \Omega_E = \frac{1}{(n-1)!} \omega^{n-1} + \frac{1}{(n-2)!} (i_\eta \omega) \wedge dE \wedge \omega^{n-1}$;
3. $\mathcal{L}_X \Omega_E = dE \wedge (i_\eta \mathcal{L}_X \Omega_E)$.

It follows in particular that the restriction of Ω_E to each regular level set $N(\mathcal{E})$ is non-vanishing and invariant under the Hamiltonian flow. Furthermore, the restriction of $i_X \Omega_E$ to the same level sets equals $\frac{1}{(n-1)!} \omega^{n-1}$.

Proof. For part (1), write $dE \wedge \Omega_E = f \Omega$ and take the interior product on both sides with η to conclude that $f \Omega_E = \Omega_E$. As Ω_E does not vanish we must have $f = 1$. For part (2), observe that

$$i_X i_\eta \omega^n = i_X (n(i_\eta \omega) \wedge \omega^{n-1}) = n\omega(\eta, X) \omega^{n-1} - n(i_\eta \omega) \wedge (i_X \omega^{n-1}).$$

But $\omega(\eta, X) = dE(\eta) = 1$ by the definition of X and η . Also $i_X \omega^{n-1} = -(n-1)dE \wedge \omega^{n-2}$. For part (3),

$$0 = \mathcal{L}_X \Omega = \mathcal{L}_X (dE \wedge \Omega_E) = dE \wedge \mathcal{L}_X \Omega_E = 0,$$

then apply interior multiplication on both sides of the equality by η . \square

In classical statistical physics, when considering and isolated macroscopic mechanical systems consisting of a large number of microscopic particles, a postulate due to Gibbs asserts that the equilibrium distribution of states of the system for a given total energy \mathcal{E} is the uniform distribution relative to Ω_E on the energy level set $N(\mathcal{E})$. This postulate is known by the name *Gibbs microcanonical ensemble*. Assigning probabilities to events, regarded as Borel subsets of $N(\mathcal{E})$, using the measure $|\Omega_E|$ only makes sense, naturally, when the total $|\Omega_E|$ -volume of a given energy level set is finite.

Proposition 10.3. Let D be a two-dimensional submanifold of $N(\mathcal{E})$ diffeomorphic to a closed disc with smooth boundary ∂D , and $T : D \rightarrow \mathbb{R}$ a smooth function. Define $\Psi(v) := \Phi_{T(v)}(v)$, where Φ_t is the Hamiltonian flow, and let D' be the image of D under Ψ . Then $\Psi^* \omega = \omega$.

Proof. Let \mathcal{T} denote the 2-dimensional set consisting of all $\Phi_t(v)$ for $v \in \partial D$ and $t \in [0, T(v)]$. We will call \mathcal{T} a *flow tube*. Note that $\int_{\mathcal{T}} \omega = 0$. In fact, at every $v \in \mathcal{T}$, the tangent space to \mathcal{T} at v is spanned by X_v and another vector ξ which is, naturally, tangent to $N(\mathcal{E})$. It follows that $\omega_v(X_v, \xi) = -dE(\xi) = 0$, hence $\omega = 0$ on \mathcal{T} . The boundary of \mathcal{T} is the union of ∂D and $-\Psi(\partial D)$ where the negative sign indicates orientation. Therefore, recalling that $\omega = d\Theta$,

$$0 = \int_{\mathcal{T}} \omega = \int_{\partial \mathcal{T}} \Theta = \int_{\partial D} \Theta - \int_{\Psi(\partial D)} \Theta = \int_{\partial D} (\Theta - \Psi^* \Theta) = \int_D (d\Theta - d\Psi^* \Theta) = \int_D (\omega - \Psi^* \omega).$$

Since the same argument applies to an arbitrary disc in D , we conclude that $\omega = \Psi^* \omega$. That is, the pull-back of ω on $\Psi(D)$ equals ω on D . \square

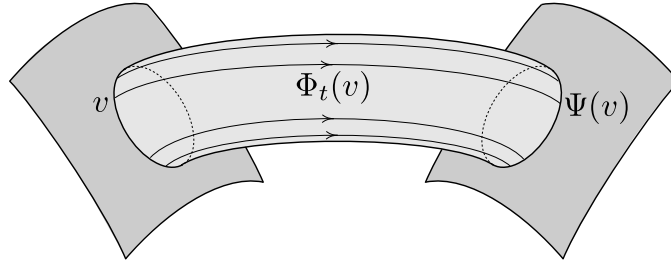


Figure 26: A flow tube used in the proof of Proposition 9.3

Recall, from Corollary 8.1 that $\omega = d\Theta$ is a symplectic form on sets of the form $N_S(\mathcal{E}) \setminus TS$. So it makes sense to define a measure $|\omega^{n-1}|$ on this set.

Proposition 10.4. Let S be a smooth hypersurface in M and \mathcal{E} a regular value of the energy function, with level set $N(\mathcal{E})$. Let $N_S(\mathcal{E})$ be the subset of $N(\mathcal{E})$ projecting into S under the base point map. Let $U = N_S(\mathcal{E}) \setminus TS$ and define $T(v) = \inf\{t > 0 : \Phi_t(v) \in N_S(\mathcal{E})\}$ for each $v \in U$, where $T(v) = +\infty$ if the set of which we are taking the infimum is empty. Let Q be the subset of U in which T is finite and define $\Psi(v) := \Phi_{T(v)}(v)$ for $v \in Q$. Then the measure $\mu := |\omega^{n-1}|$ is invariant under Ψ ; that is, $\mu(A) = \mu(\Psi^{-1}(A))$ for any Borel set $A \subset Q$.

Proof. *

\square

Proposition 10.5. Let S be an oriented smooth hypersurface in M with orientation defined by a unit normal vector field $n(q)$. At each $q \in S$ we define the reflection map $R_q(v) := v - 2\langle v, n \rangle_q n$. Note that R defines a diffeomorphism from $N_S(\mathcal{E})$ to itself. Then $R^* \Theta = \Theta$.

Proof. Note that $\pi \circ R = \pi$ and observe that $\langle v, d\pi_v \xi \rangle_q = \langle R_q(v), d\pi_v \xi \rangle_q$ for all ξ tangent to $N_S(\mathcal{E})$ at v since $d\pi_v \xi$ is tangent to S . It follows that

$$(R^* \Theta)_v(\xi) = \Theta_{R(v)}(dR_v \xi) = \langle R(v), d(\pi \circ R)_v \xi \rangle_q = \langle R(v), d\pi_v \xi \rangle_q = \langle v, d\pi_v \xi \rangle_q = \Theta_v(\xi).$$

This shows that Θ is invariant under R . \square

We would like to obtain a more concrete description of the invariant volume on $N_S(\mathcal{E}) \setminus TS$ for a hypersurface S in M in terms of the Riemannian volume form on M and the standard volume on spheres in $T_q M$. We do this next. Recall that ω defines a symplectic form on the $(2n-2)$ -dimensional space $N_S(\mathcal{E}) \setminus TS$, where S is some hypersurface in the n -dimensional manifold M . We assume that S is oriented, and let $n(q)$, $q \in S$, be a vector unit length perpendicular to $T_q S$ for each q . Then $N_S(\mathcal{E}) \setminus TS$ is a disjoint union of the two sets

$$N_S^\pm(\mathcal{E}) := \{(q, v) \in N_S(\mathcal{E}) : \pm \langle v, n \rangle_q > 0\}.$$

Note that on a neighborhood of any point q where $U(q) < \mathcal{E}$, the set $N_S^\pm(\mathcal{E})$ is diffeomorphic to a product of an open set in S and the open hemisphere $\{x = (x_1, \dots, x_n) \in S^{n-1} : \pm x_n > 0\}$. Our immediate goal is to express the invariant volume form on $N_S^\pm(\mathcal{E})$ in terms of the Riemannian volume form on S and the volume form on hemispheres. We will do this for $N_S^+(\mathcal{E})$, the negative case being similar.

Also note that, for any given value of \mathcal{E} the only allowable configurations are those q for which $\mathcal{E} - U(q) \geq 0$ because this difference is the (non-negative) kinetic energy. Therefore, it makes sense to define the function

$$h_\mathcal{E}(q) := \sqrt{2(\mathcal{E} - U(q))}$$

on the invariant set $M(\mathcal{E}) := \{q \in M : U(q) \leq \mathcal{E}\}$. Now let W be any open set in $M(\mathcal{E})$ on which the tangent bundle of M is trivial, so that it is possible to define on W a smooth family of orthonormal vector fields e_1, \dots, e_n . We do this in such a way that on $W \cap S$, if this set is non-empty, e_n is the unit normal vector denoted n above. We denote by $N_W^+(\mathcal{E})$ the subset of $N(\mathcal{E})$ projecting to W under the base-point map $\pi : N \rightarrow M$, by S^{n-1} the unit sphere in \mathbb{R}^n , and by $F_\mathcal{E} : W \times S^{n-1} \rightarrow N_W(\mathcal{E})$ the map defined by

$$F_\mathcal{E}(q, u) := \left(q, h_\mathcal{E}(q) \sum_{i=1}^n u_i e_i(q) \right).$$

We call $F_\mathcal{E}$ a *frame map*. The Riemannian volume form on M is the n -form ω^M (defined up to a sign) such that $\omega_q^M(e_1, \dots, e_n) = 1$ for any orthonormal basis $\{e_1, \dots, e_n\}$ at q . Similarly, define ω^S , for a hypersurface S in M . Let the volume form on the sphere S^{n-1} be the $(n-1)$ -form denoted by ω^{sphere} . Recall the forms Ω_E on $N(\mathcal{E})$ and $\Omega_E^S := i_X \Omega_S$ on $N_S(\mathcal{E})$ of degrees $2n-1$ and $2n-2$, respectively.

Theorem 10.1 (Invariant volume measures). For any choice of orthonormal frame over an open set $W \subset M(\mathcal{E})$ and given the frame map $F_\mathcal{E}$ defined above we have

$$F_\mathcal{E}^* \Omega_E = \pm n h_\mathcal{E}^{n-2} \omega^M \wedge \omega^{\text{sphere}}.$$

If W is a neighborhood of a point in S , we similarly have

$$F_\mathcal{E}^* \Omega_E^S = \pm \cos \theta h_\mathcal{E}^{n-1} \omega^S \wedge \omega^{\text{sphere}}$$

where $\theta(v)$ is the angle that $v \in T_q M$ makes with the normal vector $n(q)$ for $q \in S$. Apart from the unspecified signs, these expressions do not depend on the choice of local orthonormal frames.

Proof. *

□

It is helpful to give another proof of the theorem in the special, and much simpler, case of an n -dimensional billiard system in Euclidean space with 0 potential function. We use the same notation as in Exercise 8.5, where M is an n -dimensional submanifold of \mathbb{R}^n with smooth boundary and each element of TN is written as (q, v, \dot{q}, \dot{v}) .

Exercise 10.1. Let $M = \mathbb{R}^n$ with Lagrangian $L(q, v) = \frac{1}{2}|v|^2$, where $|v|^2 = v \cdot v$. Recall the vector field η from Exercise 8.5. Show the following.

1. $\Omega = \frac{1}{n!} \omega^n = (-1)^{\frac{n(n-1)}{2}} dq_1 \wedge \cdots \wedge dq_n \wedge dv_1 \wedge \cdots \wedge dv_n$
2. The interior product of ω^n by η is $i_\eta \omega^n = \frac{n}{|v|} \Theta \wedge \omega^{n-1}$.

Exercise 10.2. Let $S^{n-1} = \{v \in \mathbb{R}^n : |v| = 1\}$ be the unit sphere in \mathbb{R}^n . The volume form on S^{n-1} is

$$\omega^{\text{sphere}} = i_v (dv_1 \wedge \cdots \wedge dv_n) = \sum_{j=1}^n (-1)^j v_j dv_1 \wedge \cdots \wedge dv_{j-1} \wedge dv_{j+1} \wedge \cdots \wedge dv_n$$

where i_v indicates interior product with the vector field $\sum_j v_j \frac{\partial}{\partial v_j}$.

Exercise 10.3. Show that the form Ω_E is

$$\Omega_E = \frac{1}{(n-1)!} \frac{1}{|v|} \Theta \wedge \omega^{n-1} = (-1)^{\frac{n(n-1)}{2}} \frac{1}{|v|} dq_1 \wedge \cdots \wedge dq_n \wedge \omega^{\text{sphere}}.$$

Let us now describe the invariant volume form on the space of boundary states with energy equal to $1/2$. That is, the set of unit vectors in N with base point in the boundary of M . We denote this set by N_S^{unit} , where S stands for the boundary of M . Let $n(q)$ be the inward pointing unit normal vector to S at $q \in S$. The tangent bundle of N_S^{unit} is

$$(10.1) \quad TN_S^{\text{unit}} = \{(q, v, \dot{q}, \dot{v}) \in TN : q \in S, v \cdot \dot{v} = 0, \dot{q} \cdot n(q) = 0\}.$$

Let e_1, \dots, e_n be any orthonormal basis of \mathbb{R}^n , with dual basis denoted e_1^*, \dots, e_n^* . The dual basis is defined by the property $e_i^*(e_j) = \delta_{ij}$ where $e_i^*(e_j)$ indicates the pairing of vector and covector. Under the identification of the Horizontal subspaces in TN with tangent spaces TM , the Hamiltonian vector field $X_{(q,v)} = (q, v, v, 0)$ may be written in terms of the basis $\{e_j\}$ as $X_{(q,v)} = \sum e_j^*(v) e_j$.

Exercise 10.4. Show that, at each boundary state, the form $i_X \Omega_E$ can be expressed in terms of any orthonormal basis e_1, \dots, e_n of \mathbb{R}^n as

$$i_X \Omega_E = (-1)^{\frac{n(n+1)}{2}} \left(\sum_j (-1)^j \frac{v \cdot e_j}{|v|} e_1^* \wedge \cdots \wedge e_{j-1}^* \wedge e_{j+1}^* \wedge \cdots \wedge e_n^* \right) \wedge \omega^{\text{sphere}}.$$

By the description of TN_S^{unit} given in the above 9.1, the form between parenthesis is evaluated on vectors tangent to S . Therefore, if we use an orthonormal basis such that e_n is normal to $T_q S$, we obtain that this form (at q) reduces to

$$(-1)^n \frac{v \cdot e_n}{|v|} e_1^* \wedge \cdots \wedge e_{n-1}^* = (-1)^n \frac{v \cdot e_n}{|v|} \omega^S$$

where ω^S denotes the Riemannian volume form of S for the Riemannian metric induced on S as a hypersurface of \mathbb{R}^n . Assuming that $E = 1/2$ so that $|v| = 1$, and denoting by $n(q)$ the inward pointing unit normal vector to S at q , conclude that

$$(i_X \Omega_E)_{(q,v)} = (-1)^{\frac{n(n+3)}{2}} v \cdot n(q) \omega^S \wedge \omega^{\text{sphere}}.$$

Definition 10.2 (The billiard map). Let M be a Riemannian manifold with boundary S and $L(q, v)$ a Newtonian Lagrangian function on $N = TM$. Denote by $n(q)$ the inward pointing unit normal vector to S at q . Let $N_S \subset N$ consist of the (q, v) such that $q \in S$ and for $\epsilon \in \{+, -\}$ denote by N_S^ϵ the two components of $N_S \setminus TS$, where N_S^ϵ consists of the (q, v) such that $\epsilon \langle v, n_q \rangle > 0$. Define the reflection map $R : N_S^- \rightarrow N_S^+$ by

$$R(q, v) = (q, v - 2\langle v, n_q \rangle n_q).$$

Let Φ_t be the Hamiltonian flow on N , and for $(q, v) \in N_S^+$ let $T(q, v) = \inf\{t > 0 : \Phi_t(q, v) \in N_S\}$. We set $T = \infty$ if the set of which we are taking the infimum is empty. Let N_{billiard}^+ be the subset of N_S^+ on which T is finite, and define on N_{billiard}^+ the map $\Psi(q, v) := \Phi_{T(q,v)}(q, v)$. Finally, define the map $B : N_{\text{billiard}}^+ \rightarrow N_S^+$ by $B := R \circ \Psi$. We call B the *billiard map* of the Hamiltonian system with boundary. Then μ is invariant under the billiard map B .

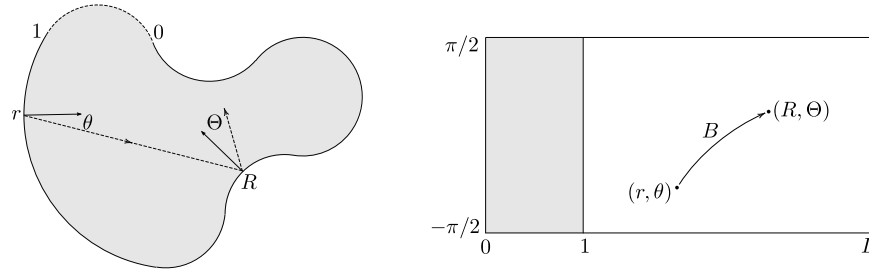


Figure 27: The billiard map B on the phase space $[0, L] \times (-\pi/2, \pi/2)$ of the two-dimensional billiard system. If we parametrize the state using the variables (r, s) , where $s = \sin \theta$, then the invariant (normalized) billiard measure is the normalized area measure $d\mu(r, s) = \frac{1}{2L} dr ds$ on the rectangle $[0, L] \times (-1, 1)$.

Corollary 10.1. We use the notations of Definition 9.2 and assume that the Lagrangian function is $L(q, v) = \frac{1}{2} \|v\|_q^2$. Define on N_S^+ the measure μ such that

$$d\mu(q, v) = v \cdot n(q) d\text{Vol}^S(q) d\text{Vol}^{\text{sphere}}(v)$$

where $d\text{Vol}^S(q)$ is the Riemannian volume element on the hypersurface S and $d\text{Vol}^{\text{sphere}}(v)$ is the volume element on the unit (hemi-)sphere in the tangent space of M at q . For billiard systems in dimension 2, $d\text{Vol}^S(q)$ is ds , where s is the variable parametrizing the boundary of the table by arclength, and $d\text{Vol}^{\text{sphere}}(v)$ is the angle measure $d\theta$, where $\theta \in (-\pi/2, \pi/2)$

is the angle that a unit vector v at q makes with the inward pointing unit normal vector $n(q)$. Thus if the billiard table has finite perimeter of length L , the probability measure $d\mu(s, \theta) = \frac{1}{2L} \cos \theta ds d\theta$ defined on the phase space $[0, L] \times (-\pi/2, \pi/2)$ is invariant under the billiard map.

Figure 28 given an interpretation of the quantity $\cos \theta \Delta s$, where $\Delta s = l$ in the figure, for the special case of a polygonal billiard table.

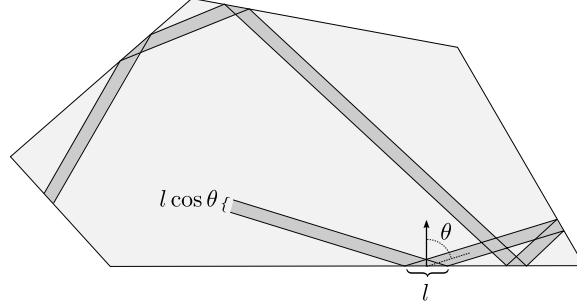


Figure 28: Illustrating the invariant billiard measure in dimension two for a polygonal billiard table. A long tape of uniform width is folded into a beam of billiard trajectories. At each collision the length l along the fold of the tape times the angle θ the tape makes with the normal vector at the collision point is constant, equal to the width. So the width is a conserved quantity of the billiard motion.

Figure 29 illustrates the invariance of the measure μ under the billiard map in dimension 2. The table is a unit square with a circular scatterer in the middle. More precise, we consider the map that gives the first return to the top side of the square of trajectories that begin at that side. Thus, for each initial condition, the return state is the image of a number of iterations of the billiard map. The initial states indicated in Figure 29 are uniformly distributed over a small rectangle in $[0, 1] \times (-\pi/2, \pi/2)$. The image of this small rectangle under the return map is widely dispersed over the phase space, but has the same measure $d\mu = \frac{1}{2} \cos \theta ds d\theta$. Note that $L = 1$ here since we are restricting attention only to the top side of the square.

Another interesting interpretation of the billiard measure in dimension 2 is shown in Figure 31. The phase space of the billiard system is in this case taken to be the rectangle $[0, 1] \times (0, \pi)$, where the angle θ is measure from the positive tangent direction to the boundary of the table, oriented counterclockwise, and the total perimeter is assumed to have length 1. As indicated in the figure, there is a natural bijection between the phase space and the 2-sphere minus the north and south poles. Regarding the sphere as the phase space of the billiard system, the invariant billiard measure μ turns out to be the normalized area measure of the sphere. In other words, the billiard map corresponds to an area preserving map of the 2-sphere.

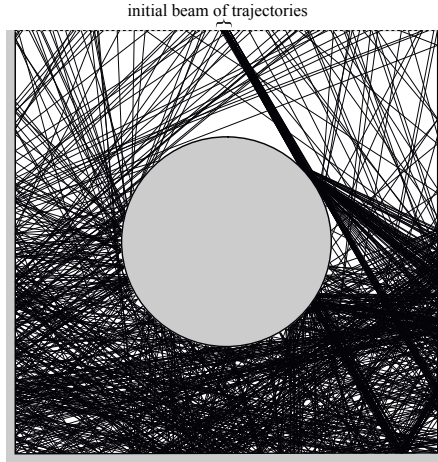


Figure 29: A beam of 10000 billiard trajectories are traced with initial position on the dashed line segment, identified with the interval $[0, 1]$, on top of the rectangular table. They are stopped at their first return to that side. The initial conditions (x, θ) are random points uniformly distributed on a phase space rectangle with $0.5 - 0.01 \leq x \leq 0.5 + 0.01$ and $-\pi/6 - 0.01 \leq \theta \leq -\pi/6 + 0.01$. The image of this small rectangle under the first return billiard map is shown in Figure 30.

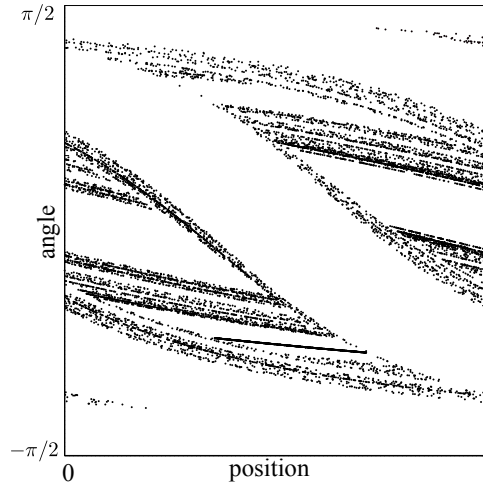


Figure 30: This scattered plot shows the end states of the first return to the dashed line segment of Figure 29 of the 10000 trajectories. The region occupied by the dots roughly represents the image under the first return map of the small rectangle in phase space of initial conditions described in the previous figures. Although the initial rectangle is greatly distorted by the map, their measures with respect to $d\mu = \frac{1}{2} \cos \theta ds d\theta$ are the same.

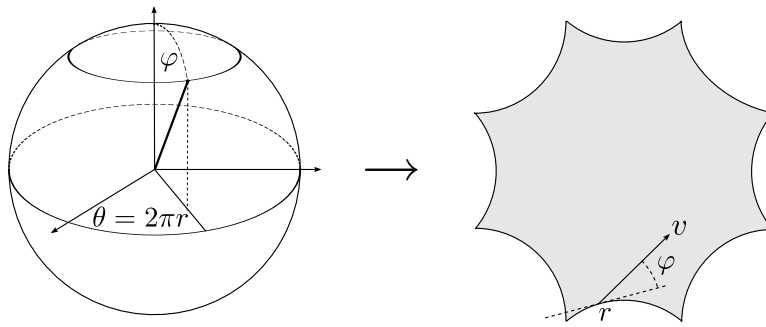


Figure 31: Assuming that the billiard table has perimeter 1, parametrized by arc-length parameter $r \in [0, 1]$, and letting $\varphi \in (0, \pi)$ denote the angle that v makes with the tangent line to the boundary of the table, then the phase space $[0, 1] \times (0, \pi)$ of the billiard system can be identified with the two-dimensional sphere (minus the north and south poles) via spherical coordinates. Under this identification the invariant probability billiard measure $\frac{1}{2} \sin \varphi \, dr \, d\varphi$ corresponds to the normalized area measure $\frac{1}{4\pi} \sin \varphi \, d\theta \, d\varphi$ of the unit two-sphere.

11 ERGODIC THEORY

Ergodic theory deals with measure theoretic issues of dynamical systems. For us it is the natural place to begin to introduce probabilistic ideas in our study of mechanical systems. To begin to see the types of questions considered in ergodic theory, let us explore a very concrete problem related to first return to a subset of the boundary of a billiard system.

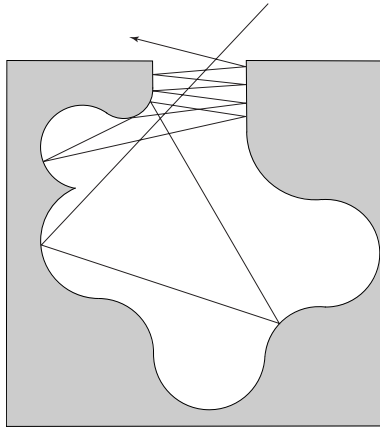


Figure 32: Light rays are flashed into a two-dimensional cave with piecewise smooth perfectly reflecting inner walls. We assume that the total area inside the cave is finite.

Consider the billiard system shown in Figure 32. We think of it as a sort of two-dimensional cave whose piecewise smooth inner walls are perfectly reflecting mirrors. The cave is open at the top; we assume that the mouth of the cave is an interval of length 1, which we identify as the unit interval $[0, 1]$. From a point r in $[0, 1]$ we flash into the cave at an angle $-\pi/2 < \theta < \pi/2$ an infinitely narrow light beam, which we think of as a single light ray. We then wait for the light ray to reemerge from the cave and register its position and angle as it leaves the cave. We may repeat this experiment as many times as we want. Here are a few questions of possible interest.

- How long, on average, does it take for the light ray to reemerge?
- How many times, on average, does a light ray bounce off the inside walls?
- What is the likely angle at which the light ray will exit the cave?
- How do these quantities depend on the internal shape of the cave?

For these questions to make sense, we need to address the following issues.

- What do we mean by “on average”?
- How do we know that light rays will reemerge in the first place?

- If light rays can get trapped inside, how likely is it to happen?
- Do we have any right to expect simple answers to these questions?

11.1 TRAPPED TRAJECTORIES

A natural first question to investigate is whether it is possible for trajectories starting outside the cave can get trapped inside and never again reemerge. We consider this problem for the specific example depicted in Figure 33.

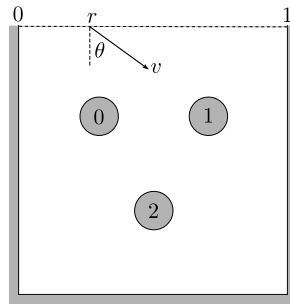


Figure 33: A cave with circular scattering walls inside. It is possible for uncountably many light trajectories starting outside the cave to get trapped inside.

Exercise 11.1. Show that there are uncountably many billiard trajectories for the system described in Figure 33 that begin outside the square and become trapped inside. In fact, given any infinite sequence a_1, a_2, a_3, \dots , where $a_j \in \{0, 1, 2\}$ such that $a_{j+1} \neq a_j$ for all j , show that there is a trajectory that bounces off the circular scatterers in the order set by the given sequence, never touching the straight sides of the table.

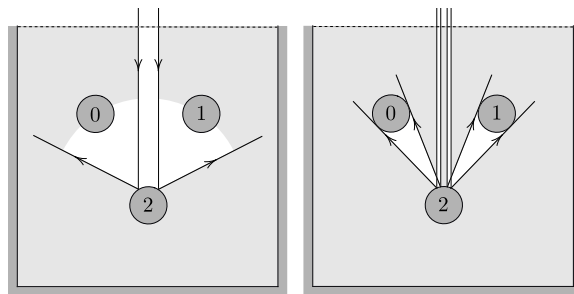


Figure 34: First two steps in the construction of a Cantor set of trapped trajectories.

11.2 WHAT IS THE PROBABILITY OF TRAPPING?

We have seen that there is a large set of initial conditions for trajectories that go into the cave and never again reemerge from it. But if we were to pick such an initial condition at random, what is the probability that we would pick one that actually leads to trapping? The answer is given by the next proposition.

Proposition 11.1. The probability of trapping is exactly 0.

But we are getting a bit ahead of ourselves. How do we define the probability of an event such as trapping in the first place? This requires choosing a probability measure on the phase space for this billiard system. It seems natural to choose a probability measure proportional to the invariant billiard measure introduced earlier. Recall that in the coordinates $(r, s = \sin \theta)$, where r is the arclength parameter along the perimeter of the boundary of the billiard region, the invariant probability is simply the normalized area measure $\frac{1}{2L} dr ds$ on the phase space rectangle $[0, L] \times (-1, 1)$. It is an axiom of classical statistical physics proposed by Josiah Willard Gibbs (sometime in the late 1800's, I believe) that probability of mechanical “events” should be computed in terms of the canonical (Liouville) measure invariant under the Hamiltonian flow, which in the present situation is the billiard (area) measure. The probability of a measurable subset $A \subset V$ is then

$$P(A) = \mu(A) = \int_A \frac{1}{2L} \cos \theta dr d\theta$$

Suppose that the entire inner perimeter of the billiard table, including the length of the open side (the dashed line in figure 35), is L . We take the length of the open side to be 1 for simplicity, so that $L > 1$.

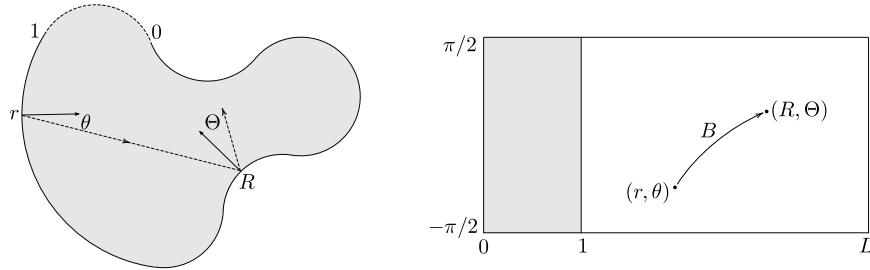


Figure 35: The billiard map B on the phase space $[0, L] \times (-\pi/2, \pi/2)$ of the two-dimensional billiard system. If we parametrize the state using the variables (r, s) , where $s = \sin \theta$, then the invariant (normalized) billiard measure is the normalized area measure $d\mu(r, s) = \frac{1}{2L} dr ds$ on the rectangle $[0, L] \times (-1, 1)$.

The contour of the table (its inner wall plus open side) is a piecewise smooth curve of length L , which we orient clockwise so as to have the open side directed in the ordinary way as a subinterval of the real line. A trajectory of the system is completely specified by giving only the sequence of coordinates of collisions between the billiard particle and the boundary of the billiard table. The direction is represented by the angle $\theta \in (-\pi/2, \pi/2)$ immediately

after collision, as shown in figure 35, and the position is given by $r \in [0, L]$. If $r \in [0, 1]$, it is understood that the billiard particle lies on the open side, in which case θ is the angle of reflection after bouncing off an imaginary flat wall placed between 0 and 1.

We write $V = [0, L] \times (-\pi/2, \pi/2)$ and call this set the *state space* (or phase space) of the billiard system. Successive collisions are described by a map

$$B : (r, \theta) \rightarrow (R, \Theta)$$

on V , as shown in figure 35. B is not generally continuous even if the boundary contour is smooth, but is a measurable (Borel) map. The set of initial billiard states will be written as $E = [0, 1] \times (-\pi/2, \pi/2) \subset V$. A trajectory of the billiard system is thus represented by a sequence

$$\xi \in E, B(\xi), B^2(\xi), B^3(\xi), \dots \in V.$$

Invariance of the probability measure P amounts to the property that, for an arbitrary event A ,

$$P(B^{-1}(A)) = P(A).$$

The trapping set \mathcal{T} can be described as the subset of states $\xi \in E$ such that $B^n(\xi)$ does not belong to E for all n . Therefore, the proposition amounts to the claim that

$$P(\mathcal{T}) = \frac{1}{2L} \int_{\mathcal{T}} \cos \theta \, dr d\theta = 0.$$

We are now ready to prove proposition 10.1. It is, in fact, an immediate corollary of the simple but fundamental fact from ergodic theory given next, known as Poincaré recurrence. To apply the recurrence theorem to the case at hand, we close down the open side with a flat wall and imagine trajectories originating at that side as having just bounced off it from the inside of the table. By this way we can assign a history trajectory to each billiard state in E .

Theorem 11.1 (Poincaré recurrence). Let $B : V \rightarrow V$ be a measure preserving transformation of a probability space V . Let P be the invariant probability measure on V and let E be a subset of V such that $P(E) > 0$. Then the trajectories starting from E that never return to E form a set of zero probability.

Proof. For $N \geq 0$, let $E_N = \bigcup_{n=N}^{\infty} B^{-n}E$. This is the set of initial conditions in V whose trajectories eventually hit E after N collisions. Then $F = E \cap \bigcap_{N=0}^{\infty} E_N$ is the set of initial conditions in E whose trajectories return to E infinitely often. In other words, if $\xi \in F$, there is a sequence $0 < n_1 < n_2 < \dots$ such that $B^{n_i}(\xi) \in E$ for all i . Notice that for all i we have $B^{n_i}(\xi) \in F$ since $B^{n_i}(\xi)$ lies in E and returns to E infinitely many times under the iterations $B^{n_j - n_i}$, for all j . We claim that $P(F) = P(E)$. Since $B^{-1}(E_N) = E_{N+1}$, by invariance of the measure under B we have $P(E_N) = P(E_{N+1})$ for all N , so $P(E_N) = P(E_0)$ for all N . Therefore, $P(F) = P(E \cap E_0) = P(E)$ since $E \subset E_0$. \square

11.3 ERGODICITY

We have found that billiard particles originating at the open side of the table will return to it with probability exactly equal to 1, so it makes sense to ask about averages.

We now add one important dynamical assumption that relates to the shape of the billiard table. We assume that (after closing the billiard table by adding a flat lid at the interval $[0, 1]$) the billiard transformation B is *ergodic*.

Definition 11.1. Let $B : V \rightarrow V$ be a measurable map on a probability space V . Let A be a subset of V such that $B^{-1}A = A$ (so that B maps A to itself). We say that A is an invariant set for B . The transformation is said to be ergodic with respect to the probability measure P if $P(A)$ can only take the values 0 or 1, for any invariant measurable A .

In other words, it is not possible to partition V into invariant subsets without one of the subsets corresponding to an impossible event (i.e., having zero probability).

It can be shown, although it is not an easy fact, that the map B for billiard tables consisting of disc scatterers in a rectangle is ergodic. (Such billiards were proven by Sinai to be ergodic). The return map to $E = [0, 1] \times (-\pi/2, \pi/2)$ (the phase space of the open side in our examples) is also ergodic. Although hard to establish, the ergodicity property is ubiquitous. In any event, we assume that the billiard systems in this discussion are ergodic.

11.4 AVERAGES

Ergodicity implies, as we see below, that the time spent by a typical trajectory in a subset of the phase space, $A \subset V$, equals $P(A)$, where P is the invariant probability measure with respect to which B is ergodic. This is the kind of statistical regularity that allows us to obtain the value of such quantities as the mean return time to the open side of the billiard table.

But first, let us review some notation and introduce some more. We have so far assumed that the length of the open side is 1. To be a little more general let this length be equal to e . Then $L > e$ and $E = [0, e] \times [-\pi/2, \pi/2]$ represents the part of the phase space for the open side. The scalar velocity of the billiard particle will be taken to be u . This value remains constant during the entire trajectory.

For each $(r, \theta) \in E$, let $S(r, \theta)$ and $N(r, \theta)$ be, respectively, the time of first return and the number of collisions before returning to the open side, counting the arrival as one collision. The entire phase space is V . For any $(r, \theta) \in V$, let $\tau(r, \theta)$ denote the time duration of free flight with initial condition (r, θ) to the point of next collision. The averages of N , S are defined by

$$\begin{aligned}\langle N \rangle_E &:= \frac{1}{2e} \int_0^e \int_{-\pi/2}^{\pi/2} N(r, \theta) \cos \theta \, d\theta \, dr; \\ \langle S \rangle_E &:= \frac{1}{2e} \int_0^e \int_{-\pi/2}^{\pi/2} S(r, \theta) \cos \theta \, d\theta \, dr.\end{aligned}$$

Similarly, the average of τ (over V) is

$$\langle \tau \rangle_V := \frac{1}{2L} \int_{-\pi/2}^{\pi/2} \tau(r, \theta) \cos \theta \, d\theta \, dr,$$

where L is the total perimeter of the billiard table, including the open side.

Theorem 11.2. Suppose that the billiard system is ergodic. Then

1. $\langle N \rangle_E = L/e$;
2. $\langle S \rangle_E = A\pi/eu$;
3. $\langle S \rangle_E = \langle N \rangle_E \langle \tau \rangle_V$.

We will discuss the proof later. As an illustration of this result, consider the two billiard tables of figure 36.

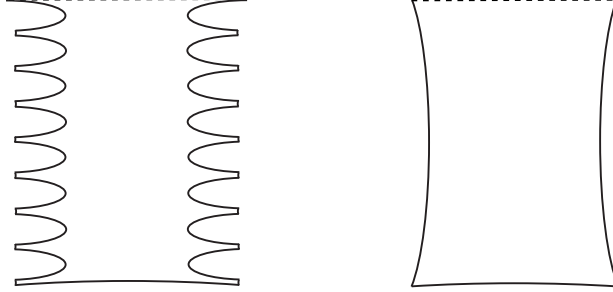


Figure 36: The average time, $\langle S \rangle_E$, is nearly the same for the two geometries shown above, although the average number of collisions, $\langle N \rangle_E$, is over three times greater for the table on the left. As the number of bumps on the boundary of the table on the left grows (assuming same height and same base), $\langle S \rangle_E$ stays nearly constant while $\langle N \rangle_E$ grows approximately linearly.

12 BIRKHOFF'S ERGODIC THEOREM

The key ingredient in the proof of theorem 10.2 is Birkhoff's ergodic theorem. This theorem, and the notion of ergodicity, belong to the foundations of classical statistical physics. The overall idea behind it is that, if the system is ergodic, almost every trajectory (i.e., with probability 1) have the same statistical behavior in the following sense: averaging quantities along trajectories gives the average of those quantities over the entire phase space. The theorem is, in fact, a general statement of the law of large numbers applied to dynamical systems with invariant probability measures. The following version of the theorem (not stated in the most general form) makes this precise. We say that a function $N : V \rightarrow \mathbb{R}$ is integrable if $\int_V |N(\xi)| dP(\xi) < \infty$.

Theorem 12.1 (Birkhoff). Let V be a probability space with probability measure P , and let $B : V \rightarrow V$ be a measure preserving transformation. Suppose that $N : V \rightarrow \mathbb{R}$ is an integrable function on V . Also assume that B is ergodic. Then, for all $\xi \in V$, except for a subset of V of zero measure, the time-average N along the orbit of ξ converges to the average of N over V ; that is,

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=0}^{n-1} N(B^i(\xi)) = \int_V N(\xi) dP(\xi).$$

The proof of Birkhoff's theorem can be found on any text in ergodic theory. I will only give here the sketch of a simple example to illustrate its use. I invite you to fill in the details. The experiment of picking a number between 0 and 1 at random (with the uniform distribution) serves as a mathematical model of flipping coins an infinite number of times, since we can regard the binary expansion of $x = 0.a_1 a_2 a_3 \dots$, $a_i \in \{0, 1\}$, as a sequence of heads and tails (say, heads = 0 and tails = 1). For this to be a sensible mathematical definition of coin tossing, we

need the average to be exactly $1/2$. We can show this by applying Birkhoff's theorem, which in this case is nothing but the law of large numbers. Let $B: [0, 1) \rightarrow [0, 1)$ be the map $B(x) = 2x - [2x]$, where $[y]$ represents the integer part of y . Notice that $B(0.a_1a_2\dots) = 0.a_2a_3\dots$. With the help of basic Fourier series you can show that B is ergodic. (Given an invariant set A , let χ_A denote its characteristic function. Now express χ_A in Fourier series and use the fact that this is an invariant function, that is, $\chi_A \circ B = \chi_A$. From this, conclude that all but the constant term in the Fourier series is 0 so χ_A is a constant function, which must, therefore, be either 0 or 1.) Let $N: [0, 1) \rightarrow \{0, 1\}$, $N(x) = a_1$, denote the value of the first binary digit of numbers in $[0, 1)$. Notice that $\int_0^1 N(x) dx = 1/2$ since $N(x)$ is 0 on the first half of the unit interval and 1 on the second half. Then the fraction of tails in a long trial of coin tosses is

$$\lim_{n \rightarrow \infty} \frac{a_1 + a_2 + \dots + a_n}{n} = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=0}^{n-1} N(B^i(x)) = \int_0^1 N(x) dx = \frac{1}{2}.$$

13 PROOF OF THEOREM 10.2

Let $B: V \rightarrow V$ be the billiard map that includes the top flat side. The first return to E is given by a map $T: E \rightarrow E$. Elements of V will be written $\xi = (r, \theta)$. Note that

$$S(\xi) = \tau(\xi) + \tau(B(\xi)) + \dots + \tau(B^{N(\xi)-1}(\xi)).$$

For each $\xi \in E$ and positive integer l , define

$$\begin{aligned} N^l(\xi) &:= N(\xi) + N(T(\xi)) + \dots + N(T^{l-1}(\xi)); \\ S^l(\xi) &:= S(\xi) + S(T(\xi)) + \dots + S(T^{l-1}(\xi)). \end{aligned}$$

Then $N^l(\xi)$ is the total number of collisions with the table boundary during the period of l returns to the flat side, and $S^l(\xi)$ is the total time during the same period. We have $\lim_{l \rightarrow \infty} N^l(\xi)/l = \langle N \rangle_E$ and $\lim_{l \rightarrow \infty} S^l(\xi)/l = \langle S \rangle_E$. Therefore, for all $\xi \in E$ but for a set of zero probability,

$$\begin{aligned} \langle N \rangle_E^{-1} &= \lim_{l \rightarrow \infty} \frac{l}{N^l(\xi)} \\ &= \lim_{l \rightarrow \infty} \frac{1}{N^l(\xi)} \sum_{i=0}^{N^l(\xi)-1} \chi_E(B^i(\xi)) \\ &= P(E) \\ &= \frac{\text{length of flat side}}{\text{total perimeter of table boundary}}. \end{aligned}$$

This shows (1). To obtain (3), start with

$$\sum_{k=0}^{N^l(\xi)-1} \tau(B^k(\xi)) = S(\xi) + S(T(\xi)) + \dots + S(T^{l-1}(\xi))$$

and average both sides over E , using T -invariance of P . This gives:

$$\left\langle \sum_{k=0}^{N^l(\xi)} \tau(B^k(\xi)) \right\rangle_E = l \langle S \rangle_E.$$

Consequently,

$$\begin{aligned} \langle S \rangle_E &= \lim_{l \rightarrow \infty} \left\langle \left(\frac{N^l(\xi)}{l} \right) \left(\frac{1}{N^l(\xi)} \sum_{k=0}^{N^l(\xi)} \tau(B^k(\xi)) \right) \right\rangle_E \\ &= \langle N \rangle_E \langle \tau \rangle_V. \end{aligned}$$

To show (2), it is convenient to first introduce the collar region U_h shown in Figure 37, where h is a small positive number.

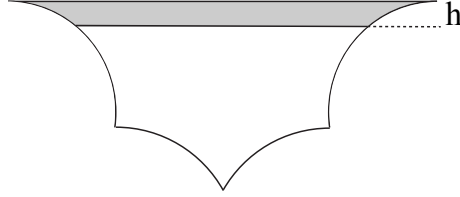


Figure 37: Define U_h as the strip of width h with the distinguished side as one of the boundary lines.

Except for a set of small measure (which goes to zero with h), the time it takes for the ray with initial condition $\xi = (x, \theta) \in E$ to traverse U_h is $\eta(\xi) = h/u \sin \theta$. An explicit integral calculation gives

$$\lim_{h \rightarrow 0} \frac{1}{h} \langle \eta \rangle_E = \pi/2u.$$

We can now conclude that, for all $\xi \in E$ except for a set of zero probability:

$$\begin{aligned} \langle S \rangle_E \frac{\text{length of flat side}}{\text{area of billiard cell}} &= \lim_{h \rightarrow 0} \lim_{m \rightarrow \infty} \left(\frac{S^m(\xi)}{m} \right) \left(\frac{1}{h S^m(\xi)} \int_0^{S^m(\xi)} \chi_{U_h}(\varphi_t(\xi)) dt \right) \\ &= \lim_{h \rightarrow 0} \lim_{l \rightarrow \infty} \frac{1}{hm} \int_0^{S^m(\xi)} \chi_{U_h}(\varphi_t(\xi)) dt \\ &= \lim_{h \rightarrow 0} \lim_{l \rightarrow \infty} \frac{1}{hm} \sum_{i=0}^{m-1} 2\eta(T^i(\xi)) \\ &= \lim_{h \rightarrow 0} \frac{2}{h} \langle \eta \rangle_E \\ &= \frac{\pi}{u}. \end{aligned}$$

This gives the average value of S claimed in (2).

14 SYSTEMS OF BILLIARD-TYPE

Although there may be plenty of trapped trajectories, the questions asked at the beginning of this section are still meaningful because, it turns out, the probability of trapping is always zero, so long as the area of the billiard table is finite.

15 RANDOM MECHANICAL SYSTEMS

16 REVIEW OF MEASURE, INTEGRATION AND HILBERT SPACES

We provide here for reference a very abbreviated review of basic measure theory and integration without any proofs. The student already familiar with this material should still skim through in order to become acquainted with our notation. A general reference for this material is [2].

Definition 16.1 (σ -Algebras and measurable maps). A non-empty family \mathcal{F} of subsets of a set \mathcal{X} is a σ -algebra if

1. If $A_i \in \mathcal{F}$, $i = 1, 2, \dots$ then $\bigcup_j^\infty A_j \in \mathcal{F}$;
2. If $A, B \in \mathcal{F}$ then the set difference $A \setminus B \in \mathcal{F}$;
3. $\mathcal{X} \in \mathcal{F}$.

Elements of \mathcal{F} are called *measurable sets*. If \mathcal{X} is a topological space, the σ -algebra of *Borel sets* of \mathcal{X} , often denoted $\mathcal{B}(\mathcal{X})$, is defined as the smallest σ -algebra containing all the open sets.

Definition 16.2 (Measurable maps). If $\mathcal{X}_1, \mathcal{X}_2$ are sets with σ -algebras $\mathcal{F}_1, \mathcal{F}_2$, respectively, a map $T : \mathcal{X}_1 \rightarrow \mathcal{X}_2$ is said to be *measurable* if the inverse image of any $A \in \mathcal{F}_2$,

$$T^{-1}(A) := \{x \in \mathcal{X}_1 : T(x) \in A\},$$

is in \mathcal{F}_1 . If \mathcal{X} is a topological space and T is a real or complex-valued function, then measurability is understood to be with respect to the Borel σ -algebra on \mathbb{R} or \mathbb{C} . For separable metric spaces, which is mainly the type of space we will encounter, the Borel σ -algebra is generated by the open (or the closed) balls.

Continuous real valued functions on a topological space are measurable. Among the measurable but not continuous functions we will typically encounter, the most ubiquitous is the indicator function of a measurable set E , denoted $\mathbb{1}_E$ and defined by

$$\mathbb{1}_E(x) := \begin{cases} 1 & \text{if } x \in E \\ 0 & \text{if } x \notin E \end{cases}$$

Functions that are linear combinations of indicator functions are called *simple* functions, or *step* functions. They have the form

$$f = \sum_{j=1}^n a_j \mathbb{1}_{A_j}.$$

Definition 16.3 (Measure). A *measure* on a (set \mathcal{X} endowed with a) σ -algebra \mathcal{F} is a function on sets $\mu : \mathcal{F} \rightarrow [0, \infty]$ such that

1. $\mu(\emptyset) = 0$;
2. If $A_i \cap A_j = \emptyset$ for all $i \neq j$ and $i, j = 1, 2, \dots$, then

$$\mu\left(\bigcup_{j=1}^{\infty} A_j\right) = \sum_{j=1}^{\infty} \mu(A_j).$$

We say that $(\mathcal{X}, \mathcal{F}, \mu)$ is a *measure space*.

Definition 16.4. A measure μ on a measurable space $(\mathcal{X}, \mathcal{F})$ is said to be

1. σ -finite if \mathcal{X} is the union of a collection of measurable sets $A_j \in \mathcal{F}$ and $\mu(A_j) < \infty$;
2. a *finite* measure if $\mu(\mathcal{X}) < \infty$;
3. a *probability measure* if $\mu(\mathcal{X}) = 1$.

The measure space $(\mathcal{X}, \mathcal{F}, \mu)$ is *complete* if whenever $E \in \mathcal{F}$, $\mu(E) = 0$, and $F \subset E$, then $F \in \mathcal{F}$.

We are mainly interested in *Borel probability measures* on metric spaces. These are, by definition, probability measures on the Borel σ -algebra $\mathcal{B}(\mathcal{X})$ of the metric space \mathcal{X} .

Proposition 16.1. Any finite Borel measure μ on a metric space \mathcal{X} is *regular*. This means that for every $A \in \mathcal{B}(\mathcal{X})$

$$\inf\{\mu(C) : C \subset A \text{ and } C \text{ closed}\} = \mu(A) = \sup\{\mu(U) : A \subset U \text{ and } U \text{ open}\}.$$

Theorem 16.1 (Tight measures). If \mathcal{X} is a complete separable metric space, then every finite Borel measure is *tight*. This means that for every $\epsilon > 0$ there exists a compact set $K \subset \mathcal{X}$ such that $\mu(\mathcal{X} \setminus K) < \epsilon$.

A tight Borel measure is also called a *Radon* measure.

Proposition 16.2. Suppose $(\mathcal{X}, \mathcal{F}, \mu)$ is complete and let $f_n : \mathcal{X} \rightarrow \mathbb{C}$ be a sequence of measurable functions such that f_n converges to f μ -almost everywhere (abbreviated μ -a.e.); that is, there exists a subset E of μ -measure zero such that for all x not in E , $f_n(x)$ converges to $f(x)$. Then f is measurable.

Theorem 16.2. If $f : \mathcal{X} \rightarrow \mathbb{C}$ is measurable, there exists a sequence $f_n : \mathcal{X} \rightarrow \mathbb{C}$ of simple functions such that $0 \leq |f_1| \leq |f_2| \leq \dots \leq |f|$ and

1. $f_n(x)$ converges to $f(x)$ for all $x \in \mathcal{X}$,
2. f_n converges uniformly to f on any set on which f is bounded.

We now define for a simple function $f = \sum_{j=1}^n a_j \mathbb{1}_{E_j}$ the integral

$$\int_{\mathcal{X}} f(x) d\mu(x) = \sum_{j=1}^n a_j \mu(E_j).$$

If f is a non-negative measurable function, we define

$$\int f(x) d\mu(x) = \sup \left\{ \int \phi d\mu : 0 \leq \phi \leq f \text{ and } \phi \text{ simple} \right\}.$$

This definition now extends to general real or complex valued functions by considering real and imaginary parts and their respective positive and negative parts.

For $p \geq 1$ let $\mathcal{L}^p(X) := \mathcal{L}^p(X, \mathcal{F}, \mu)$ denote the space of all complex valued measurable functions f on \mathcal{X} such that $\int |f|^p d\mu < \infty$. We say that $f, g \in \mathcal{L}^p(X)$ are equivalent if they agree on μ -a.e. x . This indeed defines an equivalence relation. The set of equivalence classes

$$L^p(X, \mathcal{F}, \mu) = \mathcal{L}^p(X, \mathcal{F}, \mu) / \sim$$

is a vector space. We often denote it by $L^p(\mathcal{X}, \mu)$ or simply $L^p(\mathcal{X})$. Following customary abuse of notation, we will not distinguish between \mathcal{L}^p and L^p .

Theorem 16.3. $L^p(X, \mu)$ is a complete normed vector space with the norm

$$\|f\|_p := \left(\int_{\mathcal{X}} |f(x)|^p d\mu(x) \right)^{1/p}.$$

Among the L^p spaces, L^2 is special in that the norm is derived from an inner product

$$\langle f, g \rangle := \int_{\mathcal{X}} \overline{f(x)} g(x) d\mu(x).$$

A complete inner product space is a *Hilbert space*.

Theorem 16.4. Let f_1, f_2, \dots be a sequence of functions in $L^1(\mathcal{X}, \mu)$.

1. (Monotone convergence) If $0 \leq f_1 \leq f_2 \leq \dots$ and $f = \lim_{n \rightarrow \infty} f_n$ then $f \in L^1(\mathcal{X}, \mu)$ if and only if $\lim_{n \rightarrow \infty} \|f_n\|_1 < \infty$, in which case $\lim_{n \rightarrow \infty} \|f - f_n\|_1 = 0$ and $\lim_{n \rightarrow \infty} \|f_n\|_1 = \|f\|_1$.
2. (Dominated convergence) If $\lim_{n \rightarrow \infty} f_n(x) = f(x)$ μ -a.e. and there exists $g \in L^1(\mathcal{X}, \mu)$ with $|f_n(x)| \leq g(x)$ for μ -a.e. x and all n then $f \in L^1(\mathcal{X}, \mu)$ and $\lim_{n \rightarrow \infty} \|f - f_n\|_1 = 0$.
3. (Fatou) If $f_n \geq 0$, $n = 1, 2, \dots$ and $\liminf_{n \rightarrow \infty} \|f_n\|_1 < \infty$ then $f := \liminf_{n \rightarrow \infty} f_n \in L^1(\mathcal{X}, \mu)$ and $\|f\|_1 \leq \liminf_{n \rightarrow \infty} \|f_n\|_1$.

Definition 16.5 (Singular and absolutely continuous measures). Let μ and ν be two measures on a measure space $(\mathcal{X}, \mathcal{F})$.

1. The two measures are said to be *mutually singular* if there exists a measurable set A with $\mu(A) = 0$ and $\nu(\mathcal{X} \setminus A) = 0$. This is denoted $\mu \perp \nu$.
2. The measure ν is said to be *absolutely continuous* with respect to μ if whenever $\mu(A) = 0$ then also $\nu(A) = 0$. This is denoted $\nu \ll \mu$.

Theorem 16.5 (Radon-Nikodym). A measure ν is absolutely continuous with respect to a measure μ if and only if there exists a measurable function f so that

$$\nu(A) = \int_A f(x) d\mu(x)$$

for every measurable set A . The function f is uniquely determined almost everywhere with respect to μ and is often denoted $f = \frac{d\nu}{d\mu}$.

Theorem 16.6 (Lebesgue decomposition). Let μ and ν be two measures on $(\mathcal{X}, \mathcal{F})$. Then ν can be written uniquely as a sum $\nu = \nu_{ac} + \nu_{sing}$ where $\mu \perp \nu_{sing}$ and $\nu_{ac} \ll \mu$.

Definition 16.6 (Products of measurable spaces). Given two measurable spaces $(\mathcal{X}_i, \mathcal{F}_i)$, where $i = 1, 2$, the product σ -algebra $\mathcal{F}_1 \otimes \mathcal{F}_2$ on $\mathcal{X}_1 \times \mathcal{X}_2$ is the smallest σ -algebra of subsets of $\mathcal{X}_1 \times \mathcal{X}_2$ containing $\{A_1 \times A_2 : A_i \in \mathcal{F}_i, i = 1, 2\}$.

Theorem 16.7 (Product measure). Let μ_i be a σ -finite measure on $(\mathcal{X}_i, \mathcal{F}_i)$, $i = 1, 2$. Then there exists a unique measure $\mu_1 \otimes \mu_2$ on $(\mathcal{X}_1 \times \mathcal{X}_2, \mathcal{F}_1 \times \mathcal{F}_2)$ such that

$$(\mu_1 \times \mu_2)(A_1 \times A_2) = \mu_1(A_1)\mu_2(A_2).$$

If f is measurable on $\mathcal{X}_1 \times \mathcal{X}_2$, then

$$\int_{\mathcal{X}_1} \left[\int_{\mathcal{X}_2} |f(x_1, x_2)| d\mu_2(x_2) \right] d\mu_1(x_1) < \infty$$

if and only if $\int_{\mathcal{X}_1 \times \mathcal{X}_2} |f| d(\mu_1 \otimes \mu_2) < \infty$. If this is the case, then

$$\int_{\mathcal{X}_1 \times \mathcal{X}_2} f d(\mu_1 \otimes \mu_2) = \int_{\mathcal{X}_1} \left[\int_{\mathcal{X}_2} f d\mu_2 \right] d\mu_1.$$

Theorem 16.8 (Fubini-Tonelli). Let μ_i be a σ -finite measure on \mathcal{X}_i , $i = 1, 2$. Let f be a measurable function on $\mathcal{X}_1 \times \mathcal{X}_2$ such that one of the following integrals is finite:

$$\int_{\mathcal{X}_1} \left[\int_{\mathcal{X}_2} |f| d\mu_2 \right] d\mu_1, \quad \int_{\mathcal{X}_2} \left[\int_{\mathcal{X}_1} |f| d\mu_1 \right] d\mu_2, \quad \int_{\mathcal{X}_1 \times \mathcal{X}_2} |f| d(\mu_1 \otimes \mu_2).$$

Then

$$\int_{\mathcal{X}_1} \left[\int_{\mathcal{X}_2} f d\mu_2 \right] d\mu_1 = \int_{\mathcal{X}_2} \left[\int_{\mathcal{X}_1} f d\mu_1 \right] d\mu_2 = \int_{\mathcal{X}_1 \times \mathcal{X}_2} f d(\mu_1 \otimes \mu_2).$$

Definition 16.7 (Push-forward measure). If ν is a probability measure on a measurable space \mathcal{M} and $\pi : \mathcal{M} \rightarrow \mathcal{X}$ is a measurable function, we say that $\mu = \pi_* \nu$ is the *push-forward* of ν under π if $\mu(A) := \nu(\pi^{-1}(A))$ for every measurable set A .

Exercise 16.1 (Change of variables in integration). Let $(\mathcal{X}_i, \mathcal{F}_i)$ be measurable spaces for $i = 1, 2$ and let $T : \mathcal{X}_1 \rightarrow \mathcal{X}_2$ be a measurable map. Suppose that μ is a measure on \mathcal{X}_1 and h an integrable function on \mathcal{X}_2 with respect to the push-forward measure $T_*\mu$. Show that

$$\int_{\mathcal{X}_2} f d(T_*\mu) = \int_{\mathcal{X}_1} h \circ T d\mu.$$

Suggestion: First check the identity for indicator functions of sets, then simple functions.

Theorem 16.9 (Disintegration). Let \mathcal{M} and \mathcal{X} be two separable metric spaces. Let $\pi : \mathcal{M} \rightarrow \mathcal{X}$ be a Borel measurable function, let ν be a probability measure on \mathcal{M} , and μ the push-forward of ν under π . Then there exists a μ -almost everywhere uniquely determined family of probability measures $\{\eta_x : x \in \mathcal{X}\}$ on \mathcal{M} such that

1. the function $x \mapsto \eta_x$ is Borel measurable in the sense that $x \mapsto \eta_x(A)$ is a Borel measurable function for each Borel measurable set $A \subset \mathcal{M}$;
2. for μ -a.e. $x \in \mathcal{X}$, $\eta_x(\mathcal{M} \setminus \pi^{-1}(x)) = 0$; that is, η_x is concentrated on the fiber above x ,

3. for every Borel measurable function $f : \mathcal{M} \rightarrow [0, \infty]$,

$$\int_{\mathcal{M}} f(y) d\nu(y) = \int_{\mathcal{X}} \int_{\pi^{-1}(x)} f(y) d\eta_x(y) d\mu(x).$$

In particular, for any measurable set $A \subset \mathcal{M}$

$$\nu(A) = \int_{\mathcal{X}} \eta_x(A) d\mu(x).$$

It will often be convenient to use the notation $\mu(f)$ for the integral of a function f with respect to a measure μ . Thus $\mu(f) := \int f d\mu$.

16.1 DISCRETE TIME RANDOM DYNAMICAL SYSTEMS

Before discussing random mechanical systems specifically, let us consider the following abstract set up. Let $(\mathcal{M}, \mathcal{F}_{\mathcal{M}})$ and $(\mathcal{X}, \mathcal{F}_{\mathcal{X}})$ be measurable spaces and $\pi : \mathcal{M} \rightarrow \mathcal{X}$ a measurable map. We call the set $\mathcal{M}_x := \pi^{-1}(x)$ the *fiber* above $x \in \mathcal{X}$. For each x let η_x denote a probability measure on the fiber above x . We say that this family of measure depends measurably on x if whenever f is a measurable bounded function on \mathcal{M} , the function $x \mapsto \eta_x(f) := \int f d\eta_x$ is measurable. We refer to the family $\eta = \{\eta_x : x \in \mathcal{X}\}$ as a family of probability distributions on fibers.

Definition 16.8 (Random dynamical system). Let $\eta = \eta_x : x \in \mathcal{X}$ be a family of probability distributions on the fibers of the measurable map $\pi : \mathcal{M} \rightarrow \mathcal{X}$. Let $T : \mathcal{M} \rightarrow \mathcal{M}$ be a measurable transformation of \mathcal{M} and μ a probability measure on \mathcal{X} . We refer to the data (π, T, η, μ) as a random dynamical system on \mathcal{X} with initial probability μ , generated by the deterministic map T on \mathcal{M} .

Before giving examples, we should explain the idea Definition 15.8 attempts to capture. We think of T as the generator of a deterministic dynamical system on \mathcal{M} . A point ξ in \mathcal{M} fully specifies a trajectory of the system, which is the sequence of iterates $T^j(\xi)$. The factor \mathcal{X} may be regarded as the part of the state of the system that is accessible to observation and measurement, while the component of a state along fibers can only be known up to a probability distribution, η_x . We then define a random dynamical system on \mathcal{X} in terms of a sequence of random variables X_0, X_1, X_2, \dots taking on values in \mathcal{X} such that X_0 has probability distribution μ and a value of X_{n+1} given $X_n = x$ is sampled as follows. Pick a point in the fiber of x from the probability distribution η_x , then move this point forward using T , and finally project the image down to \mathcal{X} under π . The resulting point is a value of X_{n+1} . The probability distribution of the random $(n+1)$ st iterate X_{n+1} is then $(\pi \circ T)_* \eta_x$.

From this general set up of a random dynamical system introduced above we define a *Markov chain* with space of states \mathcal{X} as follows. Let μ be a probability measure on \mathcal{X} representing the statistical state of the (observable part of the) system at a given moment. Then the state of the system at the next iteration is given by

$$\mu \mapsto \mu P := (\pi \circ T)_* \mu \circ \eta.$$

The notation should be understood as follows. From μ and η we define a probability measure $\mu \circ \eta$ on \mathcal{M} so that for any, say L^∞ function $f : \mathcal{M} \rightarrow \mathbb{R}$

$$(\mu \circ \eta)(f) = \int_{\mathcal{M}} \eta_x(f) d\mu(x).$$

The push-forward operation on measures is defined by $T_* \nu(f) := \nu(f \circ T)$. The result is an operator P taking probability measures to probability measures, which we refer to as the *Markov operator*. When it is helpful to be more explicit we write, say, $P_{\eta, T}$ or P_η , instead of P .

The probability kernel η is the family of *transition probabilities* of the Markov chain. In keeping with standard notation, we let P act on measures (states) on the right, and on functions (observables) in the left. Thus Pf is the function such that $\mu(Pf) = (\mu P)(f)$ for all μ . It follows that

$$(Pf)(x) = \int_{\pi^{-1}(x)} f(\pi \circ T(\xi)) d\eta_x(\xi).$$

We say that η is the *disintegration* of a probability measure ν on \mathcal{M} relative to a probability μ on \mathcal{X} if $\nu = \mu \circ \eta$.

A probability measure ν on \mathcal{M} is *invariant* under T if $T_* \nu = \nu$, and a probability measure μ on \mathcal{X} is *stationary* for the random system if $\mu P = \mu$.

Proposition 16.3. Let ν be a T -invariant probability measure on the total space \mathcal{M} of the random system (π, T, η, μ) and suppose that η is the disintegration of ν with respect to $\mu := \pi_* \nu$. Then $\pi_* \nu$ is a stationary probability measure on \mathcal{X} .

Proof. This is immediate from the definitions:

$$(\pi_* \nu)P = (\pi \circ T)_* (\pi_* \nu) \circ \eta = \pi_* T_* \nu = \pi_* \nu.$$

We have used that $\pi_* (\mu \circ \eta) = \mu$. □

Let μ be a probability measure on \mathcal{X} and define the Hilbert space $L^2(\mathcal{X}, \mu)$ with inner product

$$\langle f, g \rangle := \int_{\mathcal{X}} f \bar{g} d\mu.$$

Proposition 16.4. Let (π, T, η, μ) be a random system, where T is an isomorphism (thus it has a measurable inverse) of the measure space \mathcal{M} and $\nu := \mu \circ \eta$ is T -invariant. Let $P_{\eta, T}$ be the associated Markov operator. Then $P_{\eta, T}$, regarded as an operator on $L^2(\mathcal{X}, \mu)$, has norm $\|P_{\eta, T}\| = 1$ and its adjoint is $P_{\eta, T}^* = P_{\eta, T^{-1}}$.

Proof. Jensen's inequality implies

$$\|P_{\eta, T} f\|^2 = \int_{\mathcal{X}} \left| \int_{\pi^{-1}(x)} f(\pi \circ T(\xi)) d\eta_x(\xi) \right|^2 d\mu(x) \leq \int_{\mathcal{X}} \int_{\pi^{-1}(x)} |f(\pi \circ T(\xi))|^2 d\eta_x(\xi) d\mu(x).$$

The integral on the right equals $\int_{\mathcal{M}} |f|^2 \circ \pi \circ T d\nu = \int_{\mathcal{M}} |f|^2 \circ \pi d\nu$, by T -invariance of ν . As $f \circ \pi$ is constant on fibers, this last integral is $\|f\|^2$, showing that the norm of the operator is bounded by 1. Taking $f = 1$ shows that the norm actually equals 1. To see that the adjoint equals the operator associated to the inverse map, simply observe the identity

$$\int_{\mathcal{M}} f(\pi(\xi)) \bar{g}(\pi(T(\xi))) \nu(\xi) = \int_{\mathcal{M}} f(\pi(T^{-1}(\xi))) \bar{g}(\pi(\xi)) \nu(\xi),$$

which is due to T -invariance of ν . □

16.2 COUNTABLE STATE MARKOV CHAINS AND EXTENSIONS

We consider here countable state Markov chains to illustrate our general definition of a random dynamical system. Let \mathcal{X} be a countable set, which we refer to as the *set of states*. Let $\mathcal{M} = \mathcal{X} \times \mathcal{X}$ and $\pi(x, y) = x$. Pairs $(x, y) \in \mathcal{M}$ describe *state transitions* and for a given family of probability measures $\eta = \{\eta_x : x \in \mathcal{X}\}$ the numbers $p_{xy} := \eta_x(y)$ define *transition probabilities*.

For this class of examples we define T by $T(x, y) = (y, x)$. The operator $P = P_{\eta, T}$ is fully determined by its action on probability measures supported on a single state. Thus let us

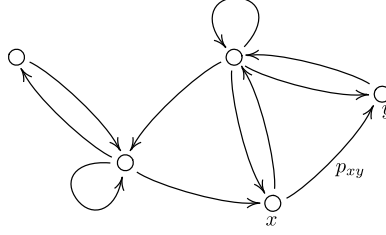


Figure 38: Directed graph representation of a Markov chain system. The nodes of the graph are the states and the arrows are the possible state transitions, labeled by the transition probabilities. Each pair of states can be connected by at most one arrow, and we only draw arrows associated to transitions with positive probability.

obtain $\delta_x P$, where δ_x is the measure assigning probability 1 to x , by pairing $\delta_x P$ with a function $f : \mathcal{X} \rightarrow \mathbb{R}$.

$$\int_{\mathcal{X}} f(x) d(\delta_x P)(x) = \int_{\mathcal{M}_x} f(\pi(T(x, y))) d\eta_x(x, y) = \sum_{y \in \mathcal{X}} p_{xy} f(y).$$

In words, the average value of a function f with respect to $\delta_x P$ is the average of f over the state that can be reached from x in one step weighted by the transition probabilities.

Let μ be a stationary measure. Thus, by definition, $\mu P = \mu$. We write $p_x := \mu(x)$ for all $x \in \mathcal{X}$. If f is any function on \mathcal{X} , then $\mu(f) = \sum_{y \in \mathcal{X}} f(y) p_y$ and

$$\begin{aligned} \int_{\mathcal{X}} f(x) d(\mu P)(x) &= \int_{\mathcal{X}} f(x) d((\pi \circ T)_* \mu \circ \eta)(x) \\ &= \int_{\mathcal{X}} \int_{\mathcal{M}_x} f(\pi \circ T(x, y)) d\eta_x(x, y) d\mu(x) = \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{X}} p_x p_{xy} f(y). \end{aligned}$$

Therefore, the identity $\mu P = \mu$ amounts to

$$(16.1) \quad p_y = \sum_{x \in \mathcal{X}} p_x p_{xy}$$

for all $y \in \mathcal{X}$. In other words, the row vector of probabilities (p_x) is an eigenvector of the transition probabilities matrix (p_{xy}) for the eigenvalue 1. This is the standard condition for a probability distribution to be stationary for a countable state Markov chain.

Exercise 16.2 (Detailed balance). For the countable state Markov chain example, show that the invariance condition $T_*(\mu \circ \eta) = \mu \circ \eta$ amounts to the set of equations

$$(16.2) \quad p_x p_{xy} = p_y p_{yx}$$

for all $x, y \in \mathcal{X}$. A countable state Markov chain with initial probability vector $p = (p_x)$ and transition matrix $P = (p_{xy})$ satisfying 15.2 is said to satisfy *detailed balance*. Show that if (p, P) satisfies detailed balance then p is a stationary probability distribution for P ; that is, Equation 15.1 holds.

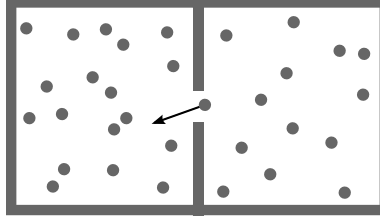


Figure 39: The Ehrenfest Markov chain is a simple model of the random dynamics of gas molecules moving between two compartments of a container.

The Ehrenfest model of gas in a divided container is a classical example of Markov chain. Gas molecules move about randomly in a box, which is divided into two equal halves by a partition. (See Figure 39.) A hole is made in the partition. Suppose there are N molecules in the box. A simple probabilistic model of this physical situation was proposed by Tatiana and Paul Ehrenfest in the early days of statistical mechanics (early 1900s) to study the second law of thermodynamics and thermodynamical equilibrium. The following is a minor variation on their model. We think of the compartments as two bowls containing chips labeled 1 through N . At each step of the (discrete time) process we choose a number between 1 and N at random with equal probabilities, then flip a coin. If the coin comes up head, the chosen chip remains in the bowl it is presently in, and if tail the chip is moved to the other bowl. The state of the system at each time step can be represented by the number of chips in the first bowl. So the set of states is $\mathcal{X} = \{0, 1, \dots, N\}$. Then the transition probabilities are

$$p_{ij} = P(X_{n+1} = j | X_n = i) = \begin{cases} i/(2N) & \text{if } j = i - 1 \\ 1/2 & \text{if } j = i \\ (N - i)/(2N) & \text{if } j = i + 1. \end{cases}$$

For example, if $N = 15$ and $X_n = 10$, then 10 out of the total 15 chips are in the first bowl. At the next step X_{n+1} can only be one of $\{9, 10, 11\}$. The probability that $X_{n+1} = 9$ is the probability that one of the 10 chips in the first bowl is chosen times the probability that the coin comes up tail. Therefore, $P(X_{n+1} = 9 | X_n = 10) = (10/15) \times (1/2)$. If the coin come up head, then the chosen chip remains in its present bowl, so $P(X_{n+1} = 10 | X_n = 10) = 1/2$. Since the only remaining transition is to $X_{n+1} = 11$ we must have $P(X_{n+1} = 11 | X_n = 10) = 5/30$, and the three probabilities add up to 1.

The transition probabilities matrix has the following form.

$$(p_{ij}) = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & \dots & 0 & 0 \\ \frac{1}{2N} & \frac{1}{2} & \frac{N-1}{2N} & 0 & \dots & 0 & 0 \\ 0 & \frac{1}{2N} & \frac{1}{2} & \frac{N-2}{2N} & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & \frac{2}{2N} & 0 \\ 0 & 0 & 0 & 0 & \dots & \frac{1}{2} & \frac{1}{2N} \\ 0 & 0 & 0 & 0 & \dots & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

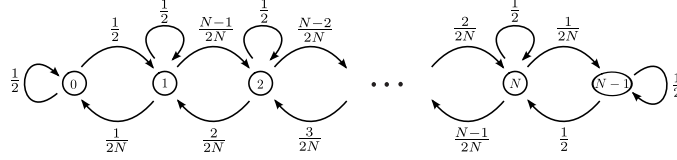


Figure 40: Transition diagram for the Ehrenfest gas model.

The directed graph for the Ehrenfest Markov chain is shown in Figure 40.

Exercise 16.3 (Ehrenfest chain). Show the following for the Ehrenfest Markov chain model.

1. The probability distribution on $\mathcal{X} = \{0, 1, \dots, N\}$ given by $p_i = \frac{1}{2^N} \binom{N}{i}$ is stationary.
2. The chain defined by (p_{ij}) and stationary probabilities (p_i) is in detailed balance.

The graph of Figure 41 shows a random trajectory of states of the Ehrenfest chain. The initial state consists of all molecules initially in one compartment of the box. The stationary distribution corresponds to a roughly equal number in each side.

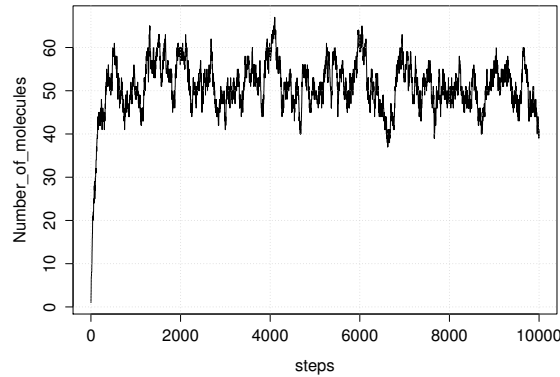


Figure 41: Number of molecules in the first compartment as a function of time, where time is being measured by the step number of the Markov chain. This illustrates the idea of thermodynamic equilibrium: the molecules quickly settle on a statistical distribution in which the two compartments have roughly an equal number of molecules. The chances that all molecules will converge back into one compartment is positive but very small.

We can build upon the simple kind of Markov chain system we have just considered to create more interesting types of random dynamical systems. Let \mathcal{S} be a measurable space

and T_1, T_2, \dots, T_k be a family of measurable maps $T_j : \mathcal{S} \rightarrow \mathcal{S}$. We denote the index set by $\mathcal{J} := \{1, \dots, k\}$, where k may be ∞ . Let $\mathcal{X} = \mathcal{S} \times \mathcal{J}$, $\mathcal{M} = \mathcal{S} \times \mathcal{J} \times \mathcal{J}$, $\pi : \mathcal{M} \rightarrow \mathcal{X}$ the projection $(u, i, j) \mapsto (u, i)$, and define the map $T : \mathcal{M} \rightarrow \mathcal{M}$ by

$$T(u, i, j) = (T_j(u), j, i).$$

Now define a family η of fiber probability measures $\eta_{u,i}(u, i, j) = p_{ij}$ for a given transition probabilities matrix (p_{ij}) on \mathcal{J} . The random dynamical system evolves as follows. At each time step the state is (u, i) , where $u \in \mathcal{S}$ and i is the index of the transformation T_i that was used in the previous time step to get to u . To update the state at the next time step, we pick j with probability p_{ij} and let the new state be $(T_j(u), j)$. In the special case when $p_{ij} = p_j$ independent of i , the second argument in (u, i) is superfluous; from state $u \in \mathcal{S}$ the system jumps to state $T_j(u)$ where j is chosen with probability p_j . For example, if T_1, T_2 are transformations of a space \mathcal{S} and $p_j = 1/2$ for $j = 1, 2$, then the random dynamical system evolves by iterating the random transformation T_I where the random index I is decided at each step by flipping a fair coin.

Stationary and invariant measures for this class of random dynamical systems are described in the next exercise.

Exercise 16.4. Consider the above extension of a Markov chain by a family of measurable maps T_j on a measurable space \mathcal{S} , $j \in \mathcal{J}$. A probability measure on $\mathcal{X} = \mathcal{S} \times \mathcal{J}$ can be written as $\mu = (\mu_i)$, $i \in \mathcal{J}$, where μ_i is a finite measure on $\mathcal{S} \times \{i\}$ (which we identify with \mathcal{S}) of total measure p_i and $\sum_i p_i = 1$. Let (p_{ij}) be the transition probabilities matrix for the Markov chain process on \mathcal{J} . Then show the following.

1. A probability measure $\mu = (\mu_i)$ on \mathcal{X} is stationary if and only if for each j ,

$$\mu_j = \sum_i p_{ij} T_{j*} \mu_i.$$

When \mathcal{S} reduces to a point, this condition reduces to $p_j = \sum_i p_i p_{ij}$ that characterizes a stationary probability distribution (p_i) of a countable state Markov chain.

2. A probability measure $\mu = (\mu_i)$ on \mathcal{X} is the push-forward under $\pi : \mathcal{M} \rightarrow \mathcal{X}$ of a T -invariant measure $\nu := \mu \circ \eta$ on \mathcal{M} if and only if for all $i, j \in \mathcal{J}$,

$$p_{ij} \mu_i = p_{ji} T_{i*} \mu_j.$$

When \mathcal{S} reduces to a point, this condition reduces $p_i p_{ij} = p_j p_{ji}$, which is the detailed balance condition for a countable state Markov chain.

A numerical example may help to give some life to these abstract definitions. Consider the random *affine transformation* T of \mathbb{R}^2 that maps (x, y) to (x', y') defined by

$$\begin{aligned} x' &= \cos(\Theta) + 0.4x \\ y' &= \sin(\Theta) - 0.4y \end{aligned}$$

where Θ is a random angle chosen from $\{\frac{2\pi j}{5} + \frac{\pi}{2} : j = 0, \dots, 4\}$ with equal probabilities. (An affine transformation is a linear transformation composed with a translation. The random map

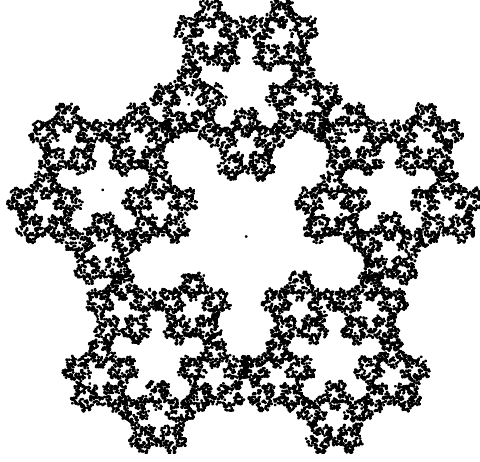


Figure 42: A finite orbit of 20000 steps, starting at the origin, of the random affine transformations of the plane defined in the text.

T first shrinks (x, y) by a factor 0.4 (the linear part) then adds a random vector as indicated (the translation part). An *orbit* or *trajectory* of this random dynamical system consists of a sequence X_0, X_1, X_2, \dots , obtained by the inductive rule: Choose an initial point X_0 then define $X_{i+1} = T(X_i)$. Since at each i the T is a possibly different (random) transformation, the sequence of points is also random. A finite orbit of this random dynamical system is shown in Figure 42. Orbits starting from different initial points look very similar, suggesting that the figure may be interpreted as a scatter plot of points sampled from a stationary probability distribution, which is likely to be unique.

Exercise 16.5. Show that if μ is a probability measure on \mathbb{R}^2 which is stationary for the random affine transformations of the example of Figure 42, then the support of μ must lie in a disc centered at the origin of radius $5/3$.

16.3 TIME REVERSIBILITY AND SYMMETRY

Let (π, T, η, μ) be a T -invariant random system, which means by definition that $\nu = \mu \circ \eta$ is a T -invariant measure so, in particular, μ is stationary. We say that the system is *time reversible* if there is a measurable isomorphism $\tilde{J} : \mathcal{M} \rightarrow \mathcal{M}$ respecting π and ν , in the sense that it maps fibers to fibers and $\tilde{J}_* \nu = \nu$, and satisfies

$$T \circ \tilde{J} = \tilde{J} \circ T^{-1}.$$

Since \tilde{J} respects π , it induces a measure preserving isomorphism $J : \mathcal{X} \rightarrow \mathcal{X}$ (for the measure μ) such that $J \circ \pi = \pi \circ \tilde{J}$. We also denote by J the induced composition operator on $L^2(\mathcal{X}, \mu)$, so $Jf := f \circ J$. Note that such J is a unitary operator on $L^2(\mathcal{X}, \mu)$. We call \tilde{J} the *time-reversing map* of the system.

Proposition 16.5. Let (π, T, η, μ) be a T -invariant random system with time-reversing map \tilde{J} , and let J be its associated unitary operator on $L^2(\mathcal{X}, \mu)$. Then $P_{\eta, T}^* = J^* P_{\eta, T} J$.

Proof. A straightforward consequence of the definitions is that

$$(P_{\eta, T} J f)(x) = \int_{\pi^{-1}} (f \circ \pi)(T^{-1} \circ \tilde{J}(\xi)) d\eta_x(\xi),$$

from which we obtain

$$\langle P_{\eta, T} J f, J g \rangle = \int_{\mathcal{M}} (f \circ \pi)(T^{-1} \circ \tilde{J}(\xi)) \overline{g}(\pi \circ \tilde{J}(\xi)) d\nu(\xi).$$

The last integral is now seen to be equal to $\int_{\mathcal{M}} f(\pi(\xi)) \overline{g}(\pi(T(\xi))) d\nu(\xi) = \langle f, P_{\eta, T} g \rangle$ by using the invariance of ν under \tilde{J} and T . \square

We say that $\tilde{S}: \mathcal{M} \rightarrow \mathcal{M}$ is an *automorphism*, or a *symmetry* of the random system if it is a measurable isomorphism commuting with T that respects π and $\nu = \mu \circ \eta$. Thus \tilde{S} covers a measure preserving isomorphism of \mathcal{X} , which we denote by S .

Definition 16.9. The T -invariant, time reversible random system (π, T, η, μ) with time reversing map \tilde{J} will be called *symmetric* if there exists an automorphism \tilde{S} whose induced map S on \mathcal{X} coincides with the map J induced from \tilde{J} .

Proposition 16.6. Let (π, T, η, μ) be a symmetric (hence time-reversible and T -invariant) random system. Then the Markov operator $P_{\eta, T}$ is self-adjoint. In particular, $P_{\eta, T^{-1}} = P_{\eta, T}$.

Proof. Given Proposition 15.5, it is enough to verify that $P_{\eta, T}$ commutes with the operator J . Keeping in mind that $J = S$, $T \circ \tilde{S} = \tilde{S} \circ T$, and that ν is \tilde{S} -invariant, we obtain

$$\begin{aligned} \int_{\mathcal{M}} f(J \circ \pi \circ T(\xi)) \overline{g}(\pi(\xi)) d\nu(\xi) &= \int_{\mathcal{M}} f(\pi \circ \tilde{S} \circ T(\xi)) \overline{g}(\pi(\xi)) d\nu(\xi) \\ &= \int_{\mathcal{M}} f(\pi \circ T(\xi)) \overline{g}(\pi \circ \tilde{S}^{-1}(\xi)) d\nu(\xi) \\ &= \int_{\mathcal{M}} f(\pi \circ T(\xi)) \overline{g}(J^{-1} \circ \pi(\xi)) d\nu(\xi). \end{aligned}$$

This means that $\langle P_{\eta, T} J f, g \rangle = \langle P_{\eta, T} f, J^{-1} g \rangle$. The claim follows as J is unitary. \square

Corollary 16.1. Let (π, T, η, μ) be a T -invariant random system, where T is an involution, i.e., T^2 equals the identity map on \mathcal{M} . Then the Markov operator $P_{\eta, T}$ is self-adjoint.

Proof. Since $T = T^{-1}$, the identity map on I is both a time reversing map and a symmetry of the system. \square

17 RANDOM BILLIARDS

18 DIFFUSION LIMITS

19 STOCHASTIC THERMODYNAMICS

19.1 A MODEL THERMODYNAMICAL SYSTEM

We consider in this section the simple thermodynamical system described in Figure 43.

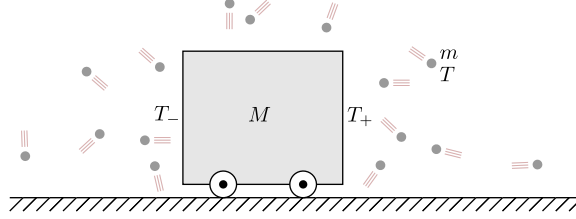


Figure 43: A particle of mass M moves without friction along a rail. It is subject to collisions with gas molecules of much smaller mass m . The temperature of the gas is T , and we assume that the vertical sides of the particle are at possibly different temperatures T_- and T_+ . We are interested in the motion of the particle.

The figure represents a particle of mass M that can move without friction along a straight line (the *rail*). The particle is immersed in a gas of particles of much smaller mass m at a certain temperature T . The constant bombardment of M by the gas particles (molecules) will cause it to move in some random fashion, which we wish to study. We assume that the two vertical sides of the particle M are kept by some unspecified mechanism at constant temperatures T_+ at the front side and T_- at the back side. It seems reasonable to expect that when $T_- = T_+$ the velocity of M behaves as Brownian motion, so that M moves somewhat erratically along the rail without a steady drift. On the other hand, we may expect that when the two temperatures on M are different, the particle will move with a definite drift that depends somehow on the two temperatures so that M will move forward if its back side is hotter than its front side. We first wish to show that this general picture is correct using a somewhat heuristic argument. Later we approach the problem of understanding the motion of M in a more systematic way by considering the particle velocity Markov chain and a diffusion limit when the ratio of masses m/M approaches 0.

We make the following assumptions and general comments concerning collisions of the gas particles with a flat wall. Let us imagine \mathbb{R}^n filled with a gas of non-interacting (non-colliding) point masses, with mass value m . The position-velocity distribution of the gas is described by a measure μ on $\mathbb{R}^n \times \mathbb{R}^n$ of the form

$$d\mu(x, v) = c \text{Vol}(x) \varrho(|v|) d\text{Vol}(v)$$

where c is for now an unspecified density constant. This means that we assume the gas to be uniformly spread over \mathbb{R}^n with anisotropic velocity. The measure of a product $A \times B$, where A is a measurable subset in position space and B a measurable subset in velocity space, is interpreted as the number of molecules in A with velocities in B . The velocity density ϱ is

assumed to be *Maxwellian* at temperature T . This means that

$$\varrho(|v|) = \left(\frac{m}{2\pi\kappa T} \right)^{n/2} e^{-\frac{m|v|^2}{2\kappa T}}$$

where κ is a constant known as the *Boltzmann constant*. Such a distribution of velocities has the property that, along any unit direction vector \mathfrak{n} , the distribution of $s = \langle v, \mathfrak{n} \rangle$ is

$$\varrho(s) = \frac{\alpha}{\sqrt{2\pi}} e^{-\frac{1}{2}(\alpha s)^2}$$

where $\alpha = \sqrt{m/\kappa T}$ has physical dimension of reciprocal of speed.

Consider now a hyperplane that moves in \mathbb{R}^n with a velocity V parallel to the plane's unit normal vector \mathfrak{n} . We call the hyperplane the *moving wall*. The hyperplane divides \mathbb{R}^n in two half-spaces. We designate one of the half-spaces to be the *positive* one, and call the side of the wall facing the positive half-space the *positive side*. We wish to know how many collisions with the gas particles happen per unit time and unit $(n-1)$ -dimensional area against the positive and the negative sides of the moving wall. We denote these numbers by $\#^+$ and $\#^-$. They will be functions of the velocity V of the wall.

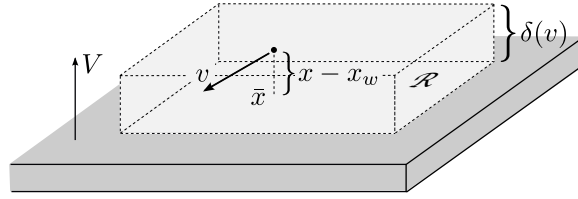


Figure 44: A thin slab in position space in which particles with velocity v will collide during the interval $[t, t + \tau]$ with a region \mathcal{R} in the positive face the moving wall.

We write position vectors as $(\bar{x}, x) = \bar{x} + x\mathfrak{n}$ where \bar{x} is the orthogonal projection of the position vector to the positive side of the moving wall, identified with \mathbb{R}^{n-1} and x is the coordinate in the direction \mathfrak{n} . Let \mathcal{R} be a subset of finite and positive area on the surface of the moving wall. We count the number of collisions with \mathcal{R} during the time interval $[t, t + \tau]$ as follows. At time t , let x and x_w be the coordinates of a particle and of points in the wall in the direction of \mathfrak{n} , respectively. Then the particle, with velocity v , will collide with the moving wall if and only if

$$0 \leq x - x_w < \langle V - v, \mathfrak{n} \rangle \tau =: \delta(v).$$

This is the condition for the plane of the wall to cross the rectilinear path of the particle during the time interval $[t, t + \tau]$. So for each velocity v , the particles with position (\bar{x}, x) at time t such that $\bar{x} \in \mathcal{R}$ that are contained in the box indicated in Figure 44—a slab with base \mathcal{R} and thickness $\delta(v)$ —will collide with that side of the moving wall. Although not all particles in the slab will hit the surface in \mathcal{R} , in the limit as τ goes to 0, we obtain $\#^+$. Note that, near the edge of the slab, there will be roughly the same number of particles that start in the slab and collide

with the wall outside of \mathcal{R} and particles that start outside of the slab (but within $\delta(v)$ of the wall) and hit the wall at a point in \mathcal{R} . This is due to the uniformity and isotropy assumptions about the gas distribution measure μ .

Note that $\delta(v)$ is only positive for $s := \langle v, \mathfrak{n} \rangle \leq S := \langle V, \mathfrak{n} \rangle$. The volume in position-velocity space corresponding to particles that hit \mathcal{R} during $[t, t + \tau]$ with velocity in $[s, s + h]$ for small h is approximately $c(S - s)A\tau\rho(s)h$, where A is the $(n - 1)$ -dimensional area of \mathcal{R} . Therefore,

$$\#^+(S) = c \int_{-\infty}^S (S - s)\rho(s) ds.$$

Using the explicit form of ρ given earlier and a change of variables in integration we write

$$\#^+(S) = \frac{c}{\sqrt{2\pi}} \frac{1}{\alpha} \int_{-\infty}^{\alpha S} (\alpha S - u) e^{-\frac{1}{2}u^2} du.$$

A similar analysis gives the following number of collisions with the opposite (negative) side of the moving wall, per unit time and unit $(n - 1)$ -dimensional area.

$$\#^-(S) = \frac{c}{\sqrt{2\pi}} \frac{1}{\alpha} \int_{\alpha S}^{\infty} (u - \alpha S) e^{-\frac{1}{2}u^2} du.$$

Exercise 19.1. Verify that the following expressions involving $\#^+(S)$ and $\#^-(S)$ hold.

1. $\#^+(S) = \frac{c}{\sqrt{2\pi}} \frac{1}{\alpha} \int_{-\infty}^{\alpha S} (\alpha S - u) e^{-\frac{1}{2}u^2} du$
2. $\#^-(S) = \frac{c}{\sqrt{2\pi}} \frac{1}{\alpha} \int_{\alpha S}^{\infty} (u - \alpha S) e^{-\frac{1}{2}u^2} du$
3. $\#^+(S) + \#^-(S) = \frac{c}{\alpha} \sqrt{\frac{2}{\pi}} \left[1 + \int_0^{\alpha S} (\alpha S - u) e^{-\frac{1}{2}u^2} du \right]$
4. $\#^+(S) - \#^-(S) = cS$
5. $\#^+(0) = \#^-(0) =: \#(0) = \frac{1}{\alpha} \frac{c}{\sqrt{2\pi}}$
6. $(\#^+(S) + \#^-(S))/\#(0) = 2 \left[1 + \int_0^{\alpha S} (\alpha S - u) e^{-\frac{1}{2}u^2} du \right]$
7. $(\#^+(S) - \#^-(S))/\#(0) = \sqrt{2\pi}\alpha S.$

Exercise 19.2. Obtain from the identities of Exercise 18.1 the estimates

$$\frac{\#^\pm(S)}{\#^\pm(0)} = 1 \pm \sqrt{\frac{\pi}{2}} \alpha S + \mathcal{O}((\alpha S)^2), \quad \frac{\#^+(S)}{\#^+(S) + \#^-(S)} = \frac{1}{2} \left(1 \pm \sqrt{\frac{\pi}{2}} \alpha S \right) + \mathcal{O}((\alpha S)^2).$$

We now return to the description of the system of Figure 43. The particle of mass M moving frictionless along the rail will be called the *Brownian particle* or, with some abuse of language, the *particle* M , and the gas particles of mass m will be called the *molecules*. Since the problem is essentially one-dimensional we let the velocities V, v be real numbers, so that $S = V$ and $s = v$. In order to obtain the random motion of the Brownian particle, we need to account for the momentum transfer due to the many collisions between the particle and the molecules. This

requires further specifying the precise characteristics of collisions as a random process. We ignore collisions with the top side of M and denote by $t_1 < t_2 < \dots$ the random times at which a collisions between M and a molecule happens. Let $\epsilon_1, \epsilon_2, \dots$ a sequence of random signs in $\{+, -\}$ indicating that the j th collision happens at the front side ($\epsilon_j = +$) or the back side ($\epsilon_j = -$). The pre-collision velocity of the molecule colliding at time t_j is denoted v_j , $j = 1, 2, \dots$, and the velocity of M just prior to the j th collision is V_j . The quantity

$$p^\pm(V) = \frac{\#^\pm(V)}{\#^+(V) + \#^-(V)} = \frac{1}{2} \left(1 \pm \sqrt{\frac{\pi}{2}} \alpha V \right) + \mathcal{O}((\alpha V)^2)$$

can be interpreted as the probability that a collision happens at the front (+) or the back (−) side given that M has velocity V .

Assumption 2. The velocity of a molecule immediately after colliding with side ϵ of M expressed relative to a frame moving with M is ϵW_ϵ , where W_ϵ is a random variable having the surface Maxwellian distribution

$$W_\epsilon \sim \frac{m}{\kappa T_\epsilon} w \exp\left(-\frac{1}{2} \frac{m w^2}{\kappa T_\epsilon}\right).$$

We assume that $t_{j+1} - t_j$, ϵ_j , $j = 1, 2, \dots$ are statistically independent (as sequences and of each other), that the W_{ϵ_j} are independent of the $t_{j+1} - t_j$ and that the v_j are independent amongst themselves and of all the other random variables, and are distributed according to $\varrho(s) = \frac{\alpha}{\sqrt{2\pi}} e^{-\frac{1}{2}(\alpha s)^2}$ where $\alpha = \sqrt{m/\kappa T}$.

If $\epsilon_j W_{\epsilon_j}$ is the post-collision velocity of a molecule at the j th collision relative to a frame moving with M , then the same velocity at a fixed frame is $v' = V_j + \epsilon_j W_{\epsilon_j}$, whereas v' is also obtained from the law of conservation of momentum: $m v' + M V_{j+1} = m v_j + M V_j$. Eliminating v' from these two equations gives the recurrence relation

$$(19.1) \quad V_{j+1} = \left(1 - \frac{m}{M}\right) V_j + \frac{m}{M} (v_j - \epsilon_j W_{\epsilon_j}).$$

Exercise 19.3. Let $\gamma := m/M$. Show that relation 18.1 implies

$$V_k = (1 - \gamma)^k V_0 + \gamma \sum_{j=1}^k (1 - \gamma)^{k-j} (v_j - \epsilon_j W_{\epsilon_j}).$$

Note that $p^\pm := \text{Prob}(\epsilon = \pm)$ should depend on the velocity V of M at the stationary regime:

$$p^\pm = E \left[\frac{\#^\pm(V)}{\#^+(V) + \#^-(V)} \right].$$

Using the approximate identities in Exercise 18.2 and taking expectations, we obtain up to first order in $E[V]$ (this step is heuristic; we elaborate on this point in the subsequent discussion)

$$(19.2) \quad p^\pm \approx \frac{1}{2} \pm \frac{\alpha}{2} \sqrt{\frac{\pi}{2}} E[V].$$

A simple integration shows that

$$E[W_{\pm}] = \int_0^{\infty} \frac{m}{\kappa T_{\pm}} w^2 \exp\left(-\frac{1}{2} \frac{mw^2}{\kappa T_{\pm}}\right) dw = \sqrt{\frac{\pi \kappa T_{\pm}}{2m}}.$$

Therefore, up to first order in $E[V]$,

$$\begin{aligned} E[\epsilon W_{\epsilon}] &= p^+ E[W_+] - p^- E[W_-] = \sqrt{\frac{\pi}{2}} \frac{1}{\alpha} \left(p^+ \sqrt{\frac{T_+}{T}} - p^- \sqrt{\frac{T_-}{T}} \right) \\ &\approx \frac{1}{2} \sqrt{\frac{\pi}{2}} \left[\frac{1}{\alpha} \left(\sqrt{\frac{T_+}{T}} - \sqrt{\frac{T_-}{T}} \right) + E[V] \left(\sqrt{\frac{T_+}{T}} + \sqrt{\frac{T_-}{T}} \right) \right] \end{aligned}$$

We wish to obtain the drift velocity EV of the Brownian particle when $T_+ \neq T_-$. Taking the expectation of the expression in Exercise 18.3 and noting that $E[v_j] = 0$ we obtain

$$E[V_k] = (1-\gamma)^k E[V_0] - \gamma \sum_{j=1}^k (1-\gamma)^{k-j} (p^+ E[W_+] - p^- E[W_-]).$$

Note that $\sum_{j=1}^k (1-\gamma)^{k-j} = [1 - (1-\gamma)^k] / \gamma$. For large k , $(1-\gamma)^k$ approaches 0. Hence, in the stationary regime as $k \rightarrow \infty$,

$$E[V] = -\gamma \sum_{j=1}^{\infty} (1-\gamma)^{j-1} E[\epsilon W_{\epsilon}] = -\frac{1}{2} \sqrt{\frac{\pi}{2}} \left[\frac{1}{\alpha} \left(\sqrt{\frac{T_+}{T}} - \sqrt{\frac{T_-}{T}} \right) + E[V] \left(\sqrt{\frac{T_+}{T}} + \sqrt{\frac{T_-}{T}} \right) \right].$$

Finally, solving for $E[V]$ and using the fact that $E[v^2] = \kappa T / m =: v_{\text{rms}}^2$ (where “rms” stands for “root mean square”), we obtain

$$E[V] = -\frac{v_{\text{rms}}}{\sqrt{\frac{8}{\pi}} + \sqrt{\frac{T_+}{T}} + \sqrt{\frac{T_-}{T}}} \left(\sqrt{\frac{T_+}{T}} - \sqrt{\frac{T_-}{T}} \right).$$

Note that if the back of the particle is hotter than the front, $T_+ < T_-$, the mean velocity of the particle is positive, and the particle moves forward. If the temperatures are equal, the mean velocity is 0. It is interesting to observe that the expected time between collisions, assuming that the surface area at the front and back of M is A , satisfies (after disregarding terms of the order $\mathcal{O}((\alpha V)^2)$)

$$E[\Delta t] = \frac{1}{A} \frac{1}{E[\#^+(V) + \#^-(V)]} = \frac{1}{A \#(0)} \frac{1}{E\left[\frac{\#^+(V) + \#^-(V)}{\#(0)}\right]} \approx \frac{1}{cA} \sqrt{\frac{\pi m}{2\kappa T}}.$$

We would like now to derive a diffusion equation for M .

20 ELEMENTS OF PROBABILITY THEORY

We begin this section with a brief overview of some classical ideas of probability theory, provided as a reference.

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a measure space equipped with a probability measure. The principle concern in classical probability theory is with real-valued measurable functions $X : \Omega \rightarrow \mathbb{R}$ which we refer to as *random variables*. We denote the integral of a random variable X over the space Ω with respect to \mathbb{P} by $\mathbb{E}(X)$ and refer to this as the *expected value* of X .

Definition 20.1. *The distribution (or law) of a random variable X is a probability measure ν on \mathbb{R} given by $\mathbb{P} \circ X^{-1}$.*

Two random variables are said to be *identically distributed* if they have the same distribution. As an aside, the notion of the distribution of a random variable hints at the idea that real-valued random variables and in turn measures on \mathbb{R} are the focus of study, while the underlying probability measure space $(\Omega, \mathcal{F}, \mathbb{P})$ is not of principal concern. One can take this as a fundamental philosophical difference between probability theory and measure theory. As an illustration of this, we note that if X is a random variable with distribution ν , then as a consequence of the change of variables theorem the integral of X is given by $\mathbb{E}(X) = \int_{\mathbb{R}} x \nu(dx)$.

One is often interested in computing expected values of powers of a random variable X . For $r \geq 1$, we call $\mathbb{E}(X^r)$ the r^{th} *moment* of X .

The notion of independence is a key hypothesis in the theorems which we discuss below.

Definition 20.2. *A collection \mathcal{A} of random variables is said to be independent if for any $k \in \mathbb{N}$ and any $x_1, \dots, x_k \in \mathbb{R}$*

$$\mathbb{P}(X_1 \leq x_1, \dots, X_k \leq x_k) = \mathbb{P}(X_1 \leq x_1) \cdots \mathbb{P}(X_k \leq x_k)$$

Exercise 20.1. *Show that if X_1, \dots, X_k are independent then $\mathbb{E}(X_1 \cdots X_k) = \mathbb{E}(X_1) \cdots \mathbb{E}(X_k)$.*

The main objects of study in the remainder of this section are sequences of real-valued random variables $(X_n)_{n \geq 1}$. For each $n \geq 1$, let $S_n = X_1 + \cdots + X_n$. We would like to understand the limiting behavior of the partial sum sequence $(S_n)_{n \geq 1}$.

When the random variables X_n are assumed to be independent and identically distributed with common distribution equal to that of a random variable X , we have the following results. The first result, the (strong) law of large numbers, is sometimes referred to as the law of averages.

Theorem 20.1 (LLN). *If $\mu = \mathbb{E}(|X|) < \infty$, then S_n/n converges \mathbb{P} -almost surely to μ .*

Proof.

□

While the above result guarantees that for large n , S_n/n will be approximately μ , \mathbb{P} almost surely, the central limit theorem addresses the size and distribution of fluctuations S_n/n might make away from μ . Put another way, if one tosses a coin 100 times, the LLN says that one should expect about 50 tosses to result in heads, but surely it is unreasonable to expect to get precisely 50 heads; the central limit theorem addresses the distribution of possible values around 50.

In order to make this precise, we must introduce the following new notion of convergence of random variables.

Definition 20.3. Let X and X_n , $n \geq 1$ be random variables with distributions ν and ν_n respectively. Then X_n is said to converge in distribution to X , often denoted $X_n \Rightarrow X$, if

$$\int_{\mathbb{R}} f d\nu_n \rightarrow \int_{\mathbb{R}} f d\nu$$

for every bounded and continuous real function f .

Before presenting the second main result, the central limit theorem, we first introduce the characteristic function of a probability measure (which one might recognize as simply the *Fourier transform* of a measure).

Definition 20.4. The characteristic function of a probability measure ν on \mathbb{R} is given by

$$\phi(t) = \int_{\mathbb{R}} e^{itx} \nu(dx)$$

for all $t \in \mathbb{R}$.

We note that if ν is the distribution of a random variable X , it makes sense to refer to ϕ as the characteristic function of X . Observe that

$$\mathbb{E}(e^{itX}) = \int_{\mathbb{R}} e^{itx} \nu(dx) = \phi(t).$$

We summarize here three fundamental properties of the characteristic function.

Proposition 20.1. If ν_1 and ν_2 have characteristic functions $\phi_1(t)$ and $\phi_2(t)$ respectively then the convolution measure $\mu_1 \star \mu_2$ has characteristic function $\phi_1(t)\phi_2(t)$.

The next exercise shows that convolutions of measures are essential to the study of sums of independent random variables. However, the convolution is often a complicated and difficult to work with operation. Nonetheless the above proposition shows that the characteristic function of a convolution is relatively simple.

Exercise 20.2. Let X_1 and X_2 be independent random variables with distributions ν_1 and ν_2 and characteristic functions ϕ_1 and ϕ_2 . Show that the random variable $X_1 + X_2$ has distribution $\nu_1 \star \nu_2$. Conclude that the characteristic function of $X_1 + X_2$ is given by the product $\phi_1\phi_2$.

The following inversion formula shows that a measure can be recovered from its characteristic function, and implies that a measure is uniquely determined by its characteristic function.

Proposition 20.2. If the probability measure ν has characteristic function ϕ and $\nu\{a\} = \nu\{b\} = 0$, then

$$\nu(a, b] = \lim_{T \rightarrow \infty} \frac{1}{2\pi} \int_{-T}^T \frac{e^{-ita} - e^{-itb}}{it} \phi(t) dt.$$

The third key property of characteristic functions shows that convergence in distribution of random variables reduces to pointwise convergence of real-valued functions.

Theorem 20.2 (Lévy Continuity Theorem). If (X_n) is a sequence of random variables with characteristic functions $\phi_n(t)$, then X_n converges in distribution to a random variable X if and only if $\phi_n(t)$ converges pointwise to the characteristic function of X for each $t \in \mathbb{R}$.

The above observations are key to the proof of the following result.

Theorem 20.3 (CLT). *Let $\sigma^2 = \mathbb{E}((X - \mu)^2)$ and $\mu = \mathbb{E}(X)$. If $\sigma^2 < \infty$, then $\sqrt{n}(S_n/n - \mu)$ converges in distribution to a normal random variable with mean 0 and variance σ^2 .*

Proof. Show that the characteristic function of $\sqrt{n}(S_n/n - \mu)$ converges pointwise to the characteristic function of a normal random variable with mean 0 and variance σ^2 and apply the Lévy continuity theorem. \square

21 GENERALIZED CENTRAL LIMIT THEOREMS

As in the previous section, the main objects of study here are sequences of random variables which are identically distributed with a common distribution equal to that of a random variable X . For clarity of exposition, we will suppose $\mathbb{E}(X) = 0$. It should be noted that this is not a particularly restrictive condition because for any random variable X with $\mathbb{E}|X| < \infty$ one can define $Y = X - \mathbb{E}(X)$ and observe that $\mathbb{E}(Y) = 0$.

Our goal in this section is to outline results that are similar in nature to the central limit theorem of the previous section. We hope to relax the hypotheses of finite variance and independence in such a way that the conclusion remains the same: an appropriate scaling of the partial sum sequence converges to a normal random variable.

We begin by relaxing the hypothesis of finite variance. A key idea in getting around the technical obstacle presented by infinite variance is the technique of truncation which we now discuss.

For a measurable set $A \in \mathcal{F}$, let $\mathbb{1}_A(\omega)$ denote the function that takes value 1 for $\omega \in A$ and 0 for $\omega \notin A$. For $x \in [0, \infty)$, define

$$L(x) = \mathbb{E}(X^2 \mathbb{1}_{\{|X| \leq x\}}).$$

We note that for each $x \in (0, \infty)$ we have $X^2 \mathbb{1}_{\{|X| \leq x\}}$ is a bounded function and so it's trivially true that $L(x)$ is finite. Now, if the growth of $L(x)$ as $x \rightarrow \infty$ is slow enough, a central limit theorem with a slightly different scaling of S_n will hold. The following definition makes precise what we mean by slow enough.

Definition 21.1. *A function $g : (0, \infty) \rightarrow (0, \infty)$ is said to be slowly varying if for all $a > 0$, $\frac{g(ax)}{g(x)} \rightarrow 1$ as $x \rightarrow \infty$.*

Theorem 21.1 (CLT with infinite variance). *If $L(x)$ is slowly varying, then there exists a sequence b_n with $b_n \rightarrow \infty$ and such that S_n/b_n converges in distribution to a normal random variable with mean 0 and variance 1.*

Sketch of proof. The sequence b_n above plays the role of the square root of the variance of S_n . While of course this does not make sense because S_n has infinite variance, it should be that b_n is closely associated with the function $L(x)$ which gives the variance of a single truncated summand of S_n . The assumption that L be slowly varying allows one to construct the sequence b_n so that

$$(21.1) \quad \frac{nL(b_n)}{b_n^2} \rightarrow 1.$$

More precisely, one defines $b_n = \inf\{t : nU(t)/t^2 \leq 1\}$. The following exercise justifies this definition.

Exercise 21.1. Show that if $g : (0, \infty) \rightarrow (0, \infty)$ is a slowly varying function, then for any $\delta > 0$ there exists x' such that $g(x) \leq x^\delta$ for all $x > x'$.

For each $n \geq 1$ and $1 \leq k \leq n$, define $X_{k,n} = X_k$ and $X'_{k,n} = X_k \mathbb{1}_{|X_k| \leq b_n}$. Note that $S_n = X_{1,n} + \dots + X_{n,n}$. Define

$$(21.2) \quad S'_n = X'_{1,n} + \dots + X'_{n,n}$$

and $S''_n = S_n - S'_n$. The next exercise shows S''_n is in a sense negligible.

We remark that $\mathbb{E}(S''_n{}^2) = b_n^2$.

Exercise 21.2. Show that $S''_n/b_n \rightarrow 0$ in probability and conclude that S_n/b_n converges in distribution to a normal law if S'_n/b_n does.

Given the exercise above, it only remains to show that the characteristic function of S'_n/b_n converges pointwise to the characteristic function of a standard normal law. This is a straightforward but slightly technical computation. \square

The hypothesis that the sequence (X_n) consists of independent random variables can also be relaxed.

Definition 21.2. Let \mathcal{A} and \mathcal{B} be sigma algebras and define their ρ -mixing coefficient by

$$\rho(\mathcal{A}, \mathcal{B}) = \sup_{X \in L^2(\mathcal{A}), Y \in L^2(\mathcal{B})} \frac{\mathbb{E}(XY)}{\sqrt{\mathbb{E}(X^2)\mathbb{E}(Y^2)}},$$

where $L^2(\mathcal{A})$ denotes the class of random variables which are \mathcal{A} -measurable and have finite second moment.

Given a (possibly infinite) family of random variables \mathcal{S} , the σ -algebra generated by \mathcal{S} , denoted $\sigma(\mathcal{S})$ is the smallest σ -algebra with respect to which all random variables in \mathcal{S} are measurable.

Definition 21.3. Let (X_n) be a sequence of identically distributed random variables and let $\mathcal{F}_n^m = \sigma(X_i : n \leq i \leq m)$. The sequence is called ρ -mixing if

$$\rho_n = \sup_k \rho(\mathcal{F}_1^k, \mathcal{F}_{k+n}^\infty) \rightarrow 0, \quad \text{as } n \rightarrow \infty$$

This definition leads to the following version of the CLT.

Theorem 21.2. Let (X_n) be an identically distributed ρ -mixing sequence with $\mathbb{E}(X) = 0$ and $L(x)$ slowly varying. If $\rho_n = O(\gamma^n)$ for some $0 < \gamma < 1$, then there exists a sequence a_n such that $a_n \rightarrow \infty$ and S_n/a_n converges in distribution to a normal random variable with mean 0 and variance 1.

Sketch of proof. Let b_n be given as in Equation (20.1) and let S'_n be defined as in Equation (20.2). Let $a_n^2 = \mathbb{E}(S_n'^2)$. Use the big-small block technique. \square

22 LIMIT THEOREMS FOR RANDOM BILLIARDS IN CHANNELS

In the section that follows we consider a random billiard model of the following idealized experiment: a small amount of gas composed of point-like, non-interacting masses is injected into a (for simplicity of exposition 2-dimensional) channel whose walls are microscopically rough and the amount of outflowing gas per unit time is recorded. Possible gas transport characteristics that can be obtained from such an experiment are the mean value and higher moments of the molecular *time of escape*. The central question then is: what can these time characteristics of the gas outflow tell us about the microscopic interaction (i.e., scattering properties) between gas molecules and the surface of the plates? See Figure 45.

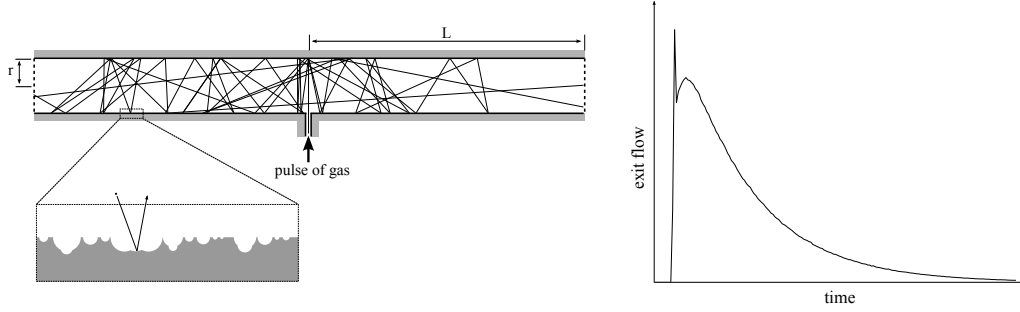


Figure 45: Idealized experiment in which a small pulse of gas is injected into a 2-dimensional channel and the gas outflow is recorded. The graph on the right represents the rate at which gas escapes. From this function it is possible to derive mean exit time of escape τ . The main problem is to relate easily measured properties of the gas outflow, such as τ , to the microscopic scattering characteristics of the channel surface.

Let us now give a precise abstract definition of our model and then describe how it relates to the above experiment.

Let \mathbb{H} denote the upper-half plane, consisting of vectors (v_1, v_2) with positive second component. Define a measurable map $v \in \mathbb{H} \mapsto \eta_v \in \mathcal{P}(\mathbb{H})$, where $\mathcal{P}(\mathbb{H})$ indicates the space of probability measures on the upper-half plane. The measurability condition is understood as follows: For every essentially bounded Borel measurable function ϕ on \mathbb{H} , the function

$$v \mapsto (P\phi)(v) := \int_{\mathbb{H}} \phi(u) d\eta_v(u)$$

is also measurable. We refer to P as the *collision operator*. Note that P specifies the transition kernel Q for a Markov chain with state space \mathbb{H} as follows: for any $v \in \mathbb{H}$ and Borel measurable set $A \subset \mathbb{H}$, let $Q(v, A) = P\mathbb{1}_A(v)$.

Let (V_n) be a Markov chain on \mathbb{H} with Markov transition kernel Q . If we suppose that microscopic structure of the rough walls of our channel is periodic and the flight of the gas particle between collisions is rectilinear at uniform speed, then we may take the Markov chain (V_n) as our model of the flight of a single gas particle. Indeed, under these assumptions, the flight of a particle is completely specified by its velocity after each wall collision.

Assumption 3. We make the following standing assumptions about the collision operator P and its associated Markov chain (V_n) .

1. The Markov chain (V_n) is positive Harris recurrent with unique stationary measure μ .
2. The operator P is self-adjoint and quasi-compact.

Let $Z(v)$ denote the horizontal displacement between channel wall collisions of a gas particle traveling with velocity v , and define $Z_n = Z(V_n)$.

Proposition 22.1. Let V_0 have distribution μ , the stationary measure of the Markov chain (V_n) . Then the sequence (Z_n) has the following properties:

1. (Z_n) is identically distributed with $\mathbb{E}(Z_n) = 0$;
2. $L(x) = \mathbb{E}(Z_n^2 \mathbb{1}_{\{|Z_n| \leq x\}})$ is slowly varying;
3. (Z_n) is ρ -mixing with $\rho_n = O(\gamma^n)$ for some $\gamma \in (0, 1)$.

The above proposition together with Theorem 20.2 shows for $S_n = Z_1 + \dots + Z_n$ there exists a scaling sequence a_n so that S_n/a_n converges in distribution to a standard normal distribution. Our interest now turns to the relationship between the scaling sequence a_n and the operator P .

Let S'_n be the truncated sequence of partial sums as defined in Equation (20.2) with truncations given by b_n as specified in Equation (20.1). The proof of Theorem 20.2 shows the sequence a_n^2 is given by $\mathbb{E}(S_n'^2)$.

Exercise 22.1. The following expression holds for all $n \geq 1$:

$$a_n^2 = n\mathbb{E}(Z_1'^2) + 2 \sum_{1 \leq i < j \leq n} \mathbb{E}(Z_i' Z_j')$$

Exercise 22.2. The sequences a_n and b_n grow at the same rate. That is, $a_n = O(b_n)$.

A priori, despite the Exercise above, there is no reason to expect that the sequence a_n/b_n converges. However, if this ratio does converge, we will see that the asymptotic variance of S_n/b_n can be expressed in terms of the spectrum of the operator P .

Assumption 4. The limit of a_n/b_n as $n \rightarrow \infty$ exists.

Proposition 22.2. Let $Z' = (Z \mathbb{1}_{\{|Z| \leq b_n\}})$ and let Π denote the projection-valued spectral measure of P given by the spectral theorem for bounded, self-adjoint operators on $L^2(\mathbb{H}, \mu)$ so that $P = \int_{-1}^1 \lambda \Pi(d\lambda)$. Let

$$(22.1) \quad \mathcal{D} = \lim_{n \rightarrow \infty} \int_{-1}^1 \frac{1+\lambda}{1-\lambda} \Pi_n(d\lambda),$$

where $\Pi_n(d\lambda)$ is the measure supported on the spectrum of P and given by $\int_{\mathbb{H}} Z'(v)(\Pi(d\lambda)Z')(v) \mu(dv)$. Assumption 4 guarantees that this limit exists and

$$(22.2) \quad \lim_{n \rightarrow \infty} \frac{a_n}{b_n} = \mathcal{D}.$$

Note that the expression above is specified precisely by P which itself is characterized by the microscopic structure of the channel walls.

Corollary 22.1. *The sequence S_n/b_n converges in distribution to a normal random variable with mean 0 and variance \mathcal{D} .*

Theorem 22.1 (Diffusion limit).

Corollary 22.2 (Mean exit times).

23 EXAMPLES

This section is devoted to computing the asymptotic variance \mathcal{D} defined in (21.1) for a few specific choices of operator P . While (21.1) makes explicit the relationship between the asymptotic variance and P , we will use the characterization of \mathcal{D} given in (21.2) to do our computations.

Before specifying P we point out some parts of the computation that can be done independently of P .

Exercise 23.1. *Show that $b_n = O(\sqrt{n \log n})$. More precisely, show that*

$$\lim_{n \rightarrow \infty} \frac{b_n}{\sqrt{n \log n}}$$

exists and call the limit \mathcal{D}_0 .

Proof. Compute $\lim_{n \rightarrow \infty} \mathbb{E}(Z_1'^2)/\log n$. □

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