Structure and Interpretation of Classical Physics

Structure and Interpretation of Classical Physics

Harold Abelson, Meinhard E. Mayer, Gerald Jay Sussman, and Jack Wisdom

This book was set by the authors using the LaTeX typesetting system and was printed and bound in the United States of America.

Library of Congress Cataloging-in-Publication Data
*****TO BE SUPPLIED*****

This book is dedicated, in respect and admiration, to everyone.

Contents

Preface

> "In almost all textbooks, even the best, this principle is presented so that it is impossible to understand." (K. Jacobi *Lectures on Dynamics*, 1842-1843). I have not chosen to break with tradition.
>
> V.I. Arnold, *Mathematical Methods of Classical Mechanics* (1980), footnote on p. 246

There has been a remarkable revival of interest in classical mechanics in recent years. We now know that there is much more to classical mechanics than previously suspected. The behavior of classical systems is surprisingly rich; derivation of the equations of motion, the focus of traditional presentations of mechanics, is just the beginning. Classical systems display a complicated array of phenomena such as non-linear resonances, chaotic behavior, and transitions to chaos.

Traditional treatments of mechanics concentrate most of their effort on the extremely small class of symbolically tractable dynamical systems. We concentrate on developing general methods for studying the behavior of systems, whether or not they have a symbolic solution. Typical systems exhibit behavior that is qualitatively different from the solvable systems and surprisingly complicated. We focus on the phenomena of motion, and we make extensive use of computer simulation to explore this motion.

Even when a system is not symbolically tractable the tools of modern dynamics allow one to extract a qualitative understanding. Rather than concentrating on symbolic descriptions, we concentrate on geometric features of the set of possible trajectories. Such tools provide a basis for the systematic analysis of numerical or experimental data.

Classical mechanics is deceptively simple. It is surprisingly easy to get the right answer with fallacious reasoning or without real understanding. Traditional mathematical notation contributes to this problem. Symbols have ambiguous meanings, which depend on context, and often even change within a given context.[1] For example, a fundamental result of mechanics is the Lagrange equations. Using traditional notation the Lagrange equations are written

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} - \frac{\partial L}{\partial q^i} = 0.$$

The Lagrangian L must be interpreted as a function of the position and velocity components q^i and $\dot{q}^i$, so that the partial derivatives make sense, but then in order for the time derivative d/dt to make sense solution paths must have been inserted into the partial derivatives of the Lagrangian to make functions of time. The traditional use of ambigous notation is convenient in simple situations, but in more complicated situations it can be a serious handicap to clear reasoning. In order that the reasoning be clear and unambiguous, we have adopted a more precise mathematical notation. Our notation is functional and follows that of modern mathematical presentations.[2]

Computation also enters into the presentation of the mathematical ideas underlying mechanics. We require that our mathematical notations be explicit and precise enough so that they can

---

[1] In his book on mathematical pedagogy [9], Hans Freudenthal argues that the reliance on ambiguous, unstated notational conventions in such expressions as $f(x)$ and $df(x)/dx$ makes mathematics, and especially introductory calculus, extremely confusing for beginning students; and he enjoins mathematics educators to use more formal modern notation.

[2] In his beautiful book *Calculus on Manifolds* (1965), Michael Spivak uses functional notation. On p.44 he discusses some of the problems with classical notation. We excerpt a particularly juicy quote:

> The mere statement of [the chain rule] in classical notation requires the introduction of irrelevant letters. The usual evaluation for $D_1(f \circ (g, h))$ runs as follows:
>
> If $f(u, v)$ is a function and $u = g(x, y)$ and $v = h(x, y)$ then
>
> $$\frac{\partial f(g(x,y), h(x,y))}{\partial x} = \frac{\partial f(u,v)}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial f(u,v)}{\partial v}\frac{\partial v}{\partial x}$$
>
> [The symbol $\partial u/\partial x$ means $\partial/\partial x \; g(x, y)$, and $\partial/\partial u \; f(u, v)$ means $D_1 f(u, v) = D_1 f(g(x, y), h(x, y))$.] This equation is often written simply
>
> $$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial f}{\partial v}\frac{\partial v}{\partial x}.$$
>
> Note that f means something different on the two sides of the equation!

be interpreted automatically, as by a computer. As a consequence of this requirement the formulas and equations that appear in the text stand on their own. They have clear meaning, independent of the informal context. For example, we write Lagrange's equations in functional notation as follows:[3]

$$D(\partial_2 L \circ \Gamma[q]) - \partial_1 L \circ \Gamma[q] = 0$$

Partial derivatives are indicated as derivatives of functions with respect to particular argument positions; $\partial_2 L$ indicates the function obtained by taking the partial derivative of the Lagrangian function L with respect to the velocity argument position. The traditional partial derivative notation, which employs a derivative with respect to a "variable," depends on context and can lead to ambiguity.[4] The partial derivatives of the Lagrangian are then explicitly evaluated along a path function q. The time derivative is taken and the Lagrange equations formed. Each step is explicit; there are no implicit substitutions.

Computational algorithms are used to communicate precisely some of the methods used in the analysis of dynamical phenomena. Expressing the methods of variational mechanics in a computer language forces them to be unambiguous and computationally effective. Computation requires us to be precise about the representation of mechanical and geometric notions as computational objects and permits us to represent explicitly the algorithms for manipulating these objects. Also, once formalized as a procedure, a mathematical idea becomes a tool that can be used directly to compute results.

Active exploration on the part of the student is an essential part of the learning experience. Our focus is on understanding the motion of systems; to learn about motion the student must actively explore the motion of systems through simulation and experiment. The exercises and projects are an integral part of the presentation.

---

[3] This is presented here without explanation, to give the flavor of the notation. The text gives a full explanation.

[4] "It is necessary to use the apparatus of partial derivatives, in which even the notation is ambiguous." From V.I. Arnold, *Mathematical Methods of Classical Mechanics* (1980), Section 47, p258. See also the footnote on that page.

That the mathematics is precise enough to be interpreted automatically allows active exploration to be extended to the mathematics. The requirement that the computer be able to interpret any expression provides strict and immediate feedback as to whether the expression is correctly formulated. Experience demonstrates that interaction with the computer in this way uncovers and corrects many deficiencies in understanding.

This book presents classical mechanics from an unusual perspective. It focuses on understanding motion rather than deriving equations of motion. It weaves recent discoveries of nonlinear dynamics throughout the presentation, rather than presenting them as an afterthought. It uses functional mathematical notation that allows precise understanding of fundamental properties of classical mechanics. It uses computation to constrain notation, to capture and formalize methods, for simulation, and for symbolic analysis.

Acknowledgments

We would like to thank the many people who have helped us develop this book and this curriculum.

Structure and Interpretation of Classical Physics

1
Lagrangian Mechanics

The subject of this book is motion, and the mathematical tools used to describe it.

Centuries of careful observations of the motions of the planets revealed regularities in those motions, allowing accurate predictions of phenomena such as eclipses and conjunctions. The effort to formulate these regularities and ultimately to understand them led to the development of mathematics and to the discovery that mathematics could be effectively used to describe aspects of the physical world. That mathematics can be used to describe natural phenomena is a remarkable fact.

When a juggler throws a pin it takes a rather predictable path and it rotates in a rather predictable way. In fact, the skill of juggling depends crucially on this predictability. It is also a remarkable discovery that the same mathematical tools used to describe the motions of the planets can be used to describe the motion of the juggling pin.

Classical mechanics describes the motion of a system of particles, subject to forces describing their interactions. Complex physical objects, such as juggling pins, can be modeled as myriad particles with fixed spatial relationships maintained by stiff forces of interaction.

There are many conceivable ways a system could move that never occur. We can imagine that the juggling pin might pause in midair or go fourteen times around the head of the juggler before being caught, but these motions do not happen. How can we distinguish motions of a system that can actually occur from other conceivable motions? Perhaps we can invent some mathematical function that allows us to distinguish realizable motions from among all conceivable motions.

The motion of a system can be described by giving the position of every piece of the system at each moment. Such a description of the motion of the system is called a configuration path; the configuration path specifies the configuration as a function of time. The juggling pin rotates as it flies through the air; the configuration of the juggling pin is specified by giving the position and orientation of the pin. The motion of the juggling pin is specified by giving the position and orientation of the pin as a function of time.

The function that we seek takes a configuration path as an input and produces some output. We want the output of this function to have some characteristic behavior when the input is a realizable path. For example, the output could be a number, and we could try to arrange that the number is zero only on realizable paths. Newton's equations of motion are of this form; at each moment Newton's differential equations must be satisfied.

However, there is a alternate strategy that provides more insight and power: we could look for a path-distinguishing function that has a minimum on the realizable paths—on nearby unrealizable paths the value of the function is higher than it is on the realizable path. This is the variational strategy: for each physical system we invent a path-distinguishing function that distinguishes realizable motions of the system by having a stationary point for each realizable path.[1] For a great variety of systems[2] realizable motions of the system can be formulated in terms of a variational principle.

Mechanics, as invented by Newton and his contemporaries, describes the motion in terms of the positions, velocities, and accelerations of each of the particles in a system. In contrast to the Newtonian formulation of mechanics, the variational formulation of mechanics describes the motion of a system in terms of aggregate quantities that are associated with the motion of the system as a whole.

In the Newtonian formulation the forces can often be written as a derivative of the potential energy of the system. The potential energy is a number that is characteristic of the arrangement of

[1] A stationary point of a function is a point where the function's value does not vary as the input is varied. Local maxima or minima are stationary points.

[2] The variational formulation successfully describes a large variety of systems. It encompasses all of the Newtonian mechanics of particles and rigid bodies. The variational formulation has also been usefully applied in the description of many other systems such as classical electrodynamics, the dynamics of inviscid fluids, and the design of mechanisms such as four-bar linkages. In addition, modern formulation of quantum mechanics and quantum field theory build on many of the same concepts. However, the variational formulation does not appear to apply to all dynamical systems. For example, there is no simple prescription to apply the variational apparatus to systems with dissipation, though in special cases variational methods still apply.

the particles in the system, and does not depend on the details of how that arrangement is specified. The motion of the system is determined by considering how the individual component particles respond to these forces. The Newtonian formulation of the equations of motion is intrinsically a particle-by-particle description.

In the variational formulation the equations of motion are formulated in terms of the difference of the kinetic energy and the potential energy. This combination, like the potential energy, is characteristic of the system as a whole and does not depend on the details of how the system is specified. So we are free to choose ways of describing the system that are easiest to work with; we are liberated from the particle-by-particle description inherent in the Newtonian formulation.

The variational formulation has numerous advantages over the Newtonian formulation. The equations of motion for those parameters that describe the state of the system are derived in the same way regardless of the choice of those parameters: the method of formulation does not depend on the choice of coordinate system. In the variational formulation there is additional freedom in choosing an appropriate coordinate system. If there are positional constraints among the particles of a system the Newtonian formulation requires that we consider the forces maintaining these constraints, whereas in the variational formulation the constraints can be built into the coordinates. The variational formulation reveals the association of conservation laws with symmetries. The variational formulation provides a framework for placing any particular motion of a system in the context of all possible motions of the system. We pursue the variational formulation, because of these advantages.

1.1 The Principle of Stationary Action

Let us suppose that for each physical system there is a path-distinguishing function that is stationary on realizable paths. We will try to deduce some of its properties.

Experience of Motion

Our ordinary experience suggests that physical motion can be described by configuration paths that are continuous and smooth.[3] We do not see the juggling pin jump from one place to another. Nor do we see the juggling pin suddenly change the way it is moving.

Our ordinary experience suggests that the motion of physical systems does not depend upon the entire history of the system. If we enter the room after the juggling pin has been thrown into the air we cannot tell when it left the juggler's hand. The juggler could have thrown the pin from a variety of places at a variety of times with the same apparent result as we walk in the door.[4] So the motion of the pin does not depend on the details of the history.

Our ordinary experience suggests that the motion of physical systems is deterministic. In fact, a small number of parameters summarize the important aspects of the history of the system and determine the future evolution of the system. For example, at any moment the position, velocity, orientation and rate of change of the orientation of the juggling pin are enough to completely determine the future motion of the pin.

Realizable Paths

From our experience of motion we develop certain expectations about realizable configuration paths. If a path is realizable, then any segment of the path is a realizable path segment. Conversely, a path is realizable if every segment of the path is a realizable path segment. The realizability of a path segment depends on all points of the path in the segment. The realizability of a path segment depends on every point of the path segment in the same way; no part of the path is special. The realizability of a path

[3] Experience with systems on an atomic scale suggests that at this scale systems do not travel along well-defined configuration paths. To describe the evolution of systems on the atomic scale we employ quantum mechanics. Here, we restrict attention to systems for which the motion is well described by a smooth configuration path.

[4] Extrapolation of the orbit of the Moon backward in time cannot determine the point at which the Moon was placed on this trajectory. To determine the origin of the Moon we must supplement dynamical evidence with other physical evidence such as chemical compositions.

segment depends only on points of the path within the segment; the realizability of a path segment is a local property.

So the path-distinguishing function aggregates some local quality of the system measured at each moment along the path segment. Each moment along the path must be treated the same way. The contributions from each moment along the path segment must be combined in a way that maintains the independence of the contributions from disjoint subsegments. One method of combination, which satisfies these requirements, is to add up the contributions, making the path-distinguishing function an integral over the path segment of some local property of the path.[5]

So we will try to arrange that the path-distinguishing function, constructed as an integral of a local property along the path, assumes an extreme value for any realizable path. Such a path-distinguishing function is traditionally called an *action* for the system. We use the word "action" to be consistent with common usage. Perhaps it would be clearer to continue to call it "path-distinguishing function," but then it would be more difficult for others to know what we were talking about.[6]

In order to pursue the agenda of variational mechanics, we must invent action functions that are stationary on the realizable trajectories of the systems we are studying. We will consider actions that are integrals of some local property of the configuration path at each moment. Let γ be the configuration-path function; $\gamma(t)$ is the configuration at time t. The action of the segment of the path γ in the time interval from t_1 to t_2 is

$$\mathcal{S}[\gamma](t_1, t_2) = \int_{t_1}^{t_2} \mathcal{F}[\gamma] \tag{1.1}$$

---

[5] We suspect that this argument can be promoted to a precise constraint on the possible ways of making this path-distinguishing function.

[6] Historically, Huygens was the first to use the term "action" in mechanics. He used the term to refer to "the effect of a motion." This is an idea that came from the Greeks. In his manuscript "Dynamica" (1690) Leibnitz enunciated a "Least Action Principle" using the "harmless action", which was the product of mass, velocity, and the distance of the motion. Leibnitz also spoke of a "violent action" in the case where things collided.

where $\mathcal{F}[\gamma]$ is a function of time that measures some local property of the path. It may depend upon the value of the function γ at that time and the value of any derivatives of γ at that time.[7]

The configuration path can be locally described at a moment in terms of the configuration, the rate of change of the configuration, and all the higher derivatives of the configuration at the given moment. Given this information the path can be reconstructed in some local interval containing that moment.[8] Local properties of paths can depend on no more than the local description of the path.

The function $\mathcal{F}[\gamma]$ measures some local property of the configuration path γ. So we can decompose $\mathcal{F}[\gamma]$ into two parts: a part that extracts a local description of the path from the path function and a part that measures some property of the local description. The method of construction of a local description of a path from a path is the same for any system; the function that measures the local property of the system depends on the particular physical system. We can write[9]

$$\mathcal{F}[\gamma] = \mathcal{L} \circ \mathcal{T}[\gamma]. \tag{1.2}$$

The function $\mathcal{T}[\gamma](t)$ takes the path γ and a time t. Its value is an ordered tuple containing the time, the configuration at that time, the rate of change of the configuration at that time, and

---

[7]Traditionally, square brackets are put around functional arguments. In this case, the square brackets remind us that the value of $\mathcal{S}$ may depend on the function γ in complicated ways, such as through its derivatives.

[8]In the case of a real valued function the value of the function and its derivatives at some point can be used to construct a power series. For sufficiently nice functions (real analytic) the power series constructed in this way converges in some interval containing the point. Not all functions can be locally represented in this way. For example, the function $f(x) = \exp(-1/x^2)$, with $f(0) = 0$, is zero and has all derivatives zero at $x = 0$, but this infinite number of derivatives is insufficient to determine the function value at any other point.

[9]Here $\circ$ denotes composition of functions: $(f \circ g)(t) = f(g(t))$. In our notation the application of $\mathcal{T}$ to its path is of higher precedence than the composition, so $\mathcal{L} \circ \mathcal{T}[\gamma] = \mathcal{L} \circ (\mathcal{T}[\gamma])$.

possibly the values of higher derivatives of the path evaluated at that time:[10]

$$\mathcal{T}[\gamma](t) = (t, \gamma(t), D\gamma(t), \ldots) \tag{1.3}$$

We refer to this tuple as the *local tuple*.

The function $\mathcal{L}$ maps a local tuple to a real number. It needs no historical information that cannot be obtained from a finite number of components of the local tuple.[11] The function $\mathcal{L}$ depends on the specific details of the physical system being investigated, but does not depend on any particular configuration path.

The advantage of this decomposition is that the local description of the path is computed by a uniform process from the configuration path, independent of the system being considered. All of the system-specific information is captured in the function $\mathcal{L}$.

We will later discover that an initial segment of the local tuple will be sufficient to determine the future evolution of the system. That a configuration and a finite number of derivatives determines the future means that there is a way of determining all of the rest of the derivatives of the path from the initial segment. The way of filling in the rest of the derivatives is the dynamics of the system.

The function $\mathcal{L}$ is called a *Lagrangian*[12] for the system, and the resulting action

$$\mathcal{S}[\gamma](t_1, t_2) = \int_{t_1}^{t_2} \mathcal{L} \circ \mathcal{T}[\gamma], \tag{1.4}$$

---

[10] The derivative of a configuration path γ can be defined in terms of how it acts on sufficiently smooth real valued functions f of configurations:

$$(D^n\gamma)(t)(f) = D^n(f \circ \gamma)(t).$$

[11] The path can be locally reconstructed from the full local tuple; that $\mathcal{L}$ depends on a finite number of components of the local tuple guarantees that it measures a local property.

[12] The classical Lagrangian plays a fundamental role in the path-integral formulation of quantum mechanics (due to Dirac and Feynman), where the complex exponential of the classical action yields the relative probability amplitude for a path. The Lagrangian is the starting point for the Hamiltonian formulation of mechanics, (to be discussed in Chapter 3) which is also essential in the Schrödinger and Heisenberg formulations of quantum mechanics, and the Boltzmann-Gibbs approach to statistical mechanics.

is called the *Lagrangian action*. Lagrangians can be found for a great variety of systems. We will see that for many systems the Lagrangian can be taken to be the difference between kinetic and potential energy. Such Lagrangians depend only on the time, the configuration, and the rate of change of the configuration. We will focus on this class of systems, but will also consider more general systems from time to time.

A realizable path of the system is to be distinguished from others by having stationary action with respect to some set of nearby unrealizable paths. Now some paths near realizable paths will also be realizable: for any motion of the juggling pin there is another that is slightly different. So when addressing the question of whether the action is stationary with respect to variations of the path we must somehow restrict the set of paths we are considering to contain only one realizable path. It will turn out that for Lagrangians that depend only on the configuration and rate of change of configuration it is enough to restrict the set of paths to those that have the same configuration at the endpoints of the path segment.

The *Principle of Stationary Action*[13] asserts that for each dynamical system we can cook up a Lagrangian such that a realizable path connecting the configurations at two times t_1 and t_2 is distinguished from all conceivable paths by the fact that the action $\mathcal{S}[\gamma](t_1, t_2)$ is stationary with respect to variations of the path. For Lagrangians that depend only on the configuration and rate of change of configuration the variations are restricted to those that preserve the configurations at t_1 and t_2.[14]

[13] The principle is often called the "Principle of Least Action" because its initial formulations spoke in terms of the action being minimized rather than the more general case of taking on a stationary value. The term "Principle of Least Action" is also commonly used to refer to a result, due to Maupertuis, Euler and Lagrange, which says that free particles move along paths for which the integral of the kinetic energy is minimized among all paths with the given endpoints. Correspondingly, the term "action" is sometimes used to refer specifically to the integral of the kinetic energy. (Actually, Euler and Lagrange used the *vis viva*, or twice the kinetic energy.)

[14] Other ways of stating the principle of stationary action make it sound teleological and mysterious. For instance, one could imagine that the system considers all possible paths from its initial configuration to its final configuration and then chooses the one with the smallest action. Indeed, the underlying vision of a purposeful, economical, and rational universe played no small part in the philosophical considerations that accompanied the initial development of

Exercise 1.1: Fermat Optics

Fermat observed that the laws of reflection and refraction could be accounted for by the following facts: Light travels in a straight line in any particular medium with a velocity that depends upon the medium. The path taken by a ray from a source to a destination through any sequence of media is a path of least total time, compared to neighboring paths. Show that these facts do imply the laws of reflection and refraction.[15]

1.2 Configuration spaces

Let us consider mechanical systems that can be thought of as composed of constituent point particles, with mass and position, but with no internal structure. Extended bodies may be thought of as composed of a large number of these constituent particles with specific spatial relationships between them. Extended bodies maintain their shape because of spatial constraints between the constituent particles. Specifying the position of all the constituent particles of a system specifies the *configuration* of the system. The existence of constraints between parts of the system, such as those which determine the shape of an extended body, means that the constituent particles cannot assume all possible positions. The set of all configurations of the system that can be assumed is called the *configuration space* of the system. The *dimension* of the configuration space is the smallest number of parameters that have to be given to completely specify a configuration. The

---

mechanics. The earliest action principle that remains part of modern physics is Fermat's Principle, which states that the path traveled by a light ray between two points is the path that takes the least amount of time. Fermat formulated this principle around 1660 and used it to derive the laws of reflection and refraction. Motivated by this, the French mathematician and astronomer Pierre-Louis Moreau de Maupertuis enunciated the Principle of Least Action as a grand unifying principle in physics. In his *Essai de cosmologie* (1750) Maupertuis appealed to this principle of "economy in nature" as evidence of the existence of God, asserting that it demonstrated "God's intention to regulate physical phenomena by a general principle of the highest perfection." For a historical perspective of Maupertuis's, Euler's, and Lagrange's roles in the formulation of the principle of least action, see [13].

[15] For reflection the angle of incidence is equal to the angle of reflection. Refraction is described by Snell's law. Snell's Law is that when light passes from one medium to another, the ratio of the sines of the angles made to the normal to the interface is the inverse of the ratio of the refractive indices of the media. The refractive index is the ratio of the speed of light in the vacuum to the speed of light in the medium.

dimension of the configuration space is also called the number of *degrees of freedom* of the system.[16]

For a single unconstrained particle it takes three parameters to specify the configuration. Thus the configuration space of a point particle is three dimensional. If we are dealing with a system with more than one point particle, the configuration space is more complicated. If there are k separate particles we need $3k$ parameters to describe the possible configurations. If there are constraints among the parts of a system the configuration is restricted to a lower dimensional space. For example, a system consisting of two point particles constrained to move in three dimensions so that the distance between the particles remains fixed has a five-dimensional configuration space.

Consider a juggling pin. The configuration of the pin is specified if we give the positions of every atom making up the pin. However, there exist more economical descriptions of the configuration. In the idealization that the juggling pin is truly rigid the distances among all the atoms of the pin remain constant. So we can specify the configuration of the pin by giving the position of a single atom, and the orientation of the pin. Using the constraints the positions of all the other constituents of the pin can be determined from this information. The dimension of the configuration space of the juggling pin is six: the minimum number of parameters that specify the position in space is three, and the minimum number of parameters that specify an orientation is also three.

As a system evolves with time the constituent particles move subject to the constraints. The motion of each constituent particle is specified by describing the changing configuration. Thus, the motion of the system may be described as evolving along a path in configuration space. The configuration path may be specified

[16] Strictly speaking the dimension of the configuration space and the number of degrees of freedom are not the same. The number of degrees of freedom is the dimension of the space of configurations that are "locally accessible." For systems with integrable constraints the two are the same. For systems with non-integrable constraints the configuration dimension can be larger than the number of degrees of freedom. For further explanation see the discussion of systems with non-integrable constraints below (Section 1.10.3). Apart from that discussion, all of the systems we will consider have integrable constraints (they are "holonomic"). This is why we have chosen to blur the distinction between the number of degrees of freedom and the dimension of the configuration space.

by a function, the configuration-path function, which gives the configuration of the system at any time.

Exercise 1.2: Degrees of Freedom

For each of the mechanical systems described below give the number of degrees of freedom of the configuration space.

a. Three juggling pins.

b. A spherical pendulum, consisting of a point mass hanging from a rigid massless rod attached to a fixed support point. The pendulum bob may move in any direction subject to the constraint imposed by the rigid rod. The mass point is subject to the uniform force of gravity.

c. A spherical double pendulum consisting of one point-mass hanging from a rigid massless rod attached to a second point-mass hanging from a second massless rod attached to a fixed support point. The mass point is subject to the uniform force of gravity.

d. A point mass sliding without friction on a rigid curved wire.

e. A top consisting of a rigid axisymmetric body with one point in the body attached to a fixed support, subject to a uniform gravitational force.

f. The same as **e**, but not axisymmetric.

1.3 Generalized coordinates

In order to be able to talk about specific configurations we need to have a set of parameters that label the configurations. The parameters that are used to specify the configuration of the system are called the *generalized coordinates*. Consider an unconstrained free particle. The configuration of the particle is specified by giving its position. This requres three parameters. The unconstrained particle has three degrees of freedom. One way to specify the position of a particle is to specify its rectangular coordinates relative to some chosen coordinate axes. The rectangular components of the position are generalized coordinates for an unconstrained particle. Or consider an ideal planar double pendulum: a point mass constrained to always be a given distance from a fixed point by a rigid rod, with a second mass that is constrained to be at a given distance from the first mass by another rigid rod, all confined to a vertical plane. The configuration is specified if the orientation of the two rods is given. This requires at least two parameters; the planar double pendulum has two degrees of freedom. One way to specify the orientation of each rod is to specify the angle it makes with the vertical. These two angles are generalized coordinates for the planar double pendulum.

The number of coordinates need not be the same as the dimension of the configuration space, though there must be at least that many. We may choose to work with more parameters than necessary, but then the parameters will be subject to constraints that restrict the system to possible configurations, that is, to elements of the configuration space.

For the planar double pendulum described above, the two angle coordinates are enough to specify the configuration. We could also take as generalized coordinates the rectangular coordinates of each of the masses in the plane, relative to some chosen coordinate axes. These are also fine coordinates, but we will have to explicitly keep in mind the constraints that limit the possible configurations to the actual geometry of the system. Sets of coordinates with the same dimension as the configuration space are easier to work with because we do not have to deal with explicit constraints among the coordinates. So for the time being we will consider only formulations where the number of configuration coordinates is equal to the number of degrees of freedom; later we will learn how to handle systems with redundant coordinates and explicit constraints.

In general, the configurations form a space M of some dimension n. The n-dimensional configuration space can be parametrized by choosing n independent coordinate functions[17] χ^i, $i = 0, \ldots, n-1$, where each χ^i is a real-valued function defined on some region of the configuration space. For a given configuration m in the configuration space M the values $\chi^i(m)$ of the coordinate functions are the generalized coordinates of the configuration. These generalized coordinates permit us to identify points of the n-dimensional configuration space with n-tuples of real numbers.[18] For any given

---

[17] We use zero-based indexing.

[18] More precisely, the generalized coordinates identify open subsets of the configuration space with open subsets of $\mathbf{R}^n$. It may require more than one set of generalized coordinates to cover the entire configuration space. For example, if the configuration space is a two-dimensional sphere, we could have one set of coordinates that maps (a little more than) the northern hemisphere to a disk, and another set that maps (a little more than) the southern hemisphere to a disk, with a strip near the equator common to both coordinate systems. A space that can be locally parametrized by smooth coordinate functions is

configuration space, there are a great variety of ways to choose generalized coordinates. Even for a single point moving without constraints, we can choose rectangular coordinates, polar coordinates, or any other coordinate system that strikes our fancy.

The motion of the system can be described by a configuration path γ mapping time to the changing configuration space point. The coordinate functions map configuration paths to generalized coordinate paths: $q^i = \chi^i \circ \gamma$. More compactly, the coordinate path function is $q = \chi \circ \gamma$. The coordinate path function q is a structured object: it is a tuple of component coordinate path functions which are indexed by superscripts:[19] $q = (q^0, \ldots, q^{n-1})$. At each instant of time t, the values $q(t) = (q^0(t), \ldots, q^{n-1}(t))$ are the generalized coordinates of a configuration.

The derivative of the coordinate path function Dq gives the rate of change of the configuration coordinates at a given time: $Dq(t)$, or in terms of components $(Dq^0(t), \ldots, Dq^{n-1}(t))$.[20] The rate of change of a generalized coordinate is called a *generalized velocity*.[21]

---

called a *differentiable manifold*. The theory of differentiable manifolds can be used to formulate a coordinate-free treatment of variational mechanics. An extensive introduction to mechanics from this perspective can be found in [3] or [7] .

[19] The use of superscripts to indicate the component of the generalized coordinate tuple is traditional, even though there is potential confusion, say, with exponents.

[20] The derivative of a function f is a function. It is denoted Df. Our notational convention is that D is a high-precedence operator. Thus D operates on the adjacent function before any other application occurs: $Df(x)$ is the same as $(Df)(x)$. In this book the dot does not indicate the differentiation operation, but sometimes $\dot{q}$ is used as the name of the function that is the derivative of the function q.

[21] The generalized velocity is a vector, and $Dq(t)$ is a coordinate representation of this vector. The generalized coordinate $q(t)$ is more properly thought of as an n-tuple of numbers rather than a vector — it is not necessarily meaningful to add or scale values of q as we do with coordinates of vectors. Even though $Dq(t)$ represents a vector, it is not meaningful to add two of them from different points of a path. We can state this in abstract language: The configuration space is a differentiable manifold M, and the generalized velocity at a point $m \in M$ represents a vector in the tangent space to M at m.

Exercise 1.3: Generalized Coordinates

For each of the systems described in Exercise 1.2 specify a system of generalized coordinates that can be used to describe the behavior of the system.

1.3.1 Lagrangians in Generalized Coordinates

The Lagrangian $\mathcal{L}$ is a function of the local tuple $\mathcal{T}[\gamma](t) = (t, \gamma(t), D\gamma(t), \ldots)$. To reexpress the Lagrangian in terms of a particular set of generalized coordinates we introduce the function $\#$ that extends the coordinate representation to the local tuple:[22]

$$\#_\chi(t, \gamma(t), D\gamma(t), \ldots) = (t, q(t), Dq(t), \ldots) . \tag{1.5}$$

The function $\#_\chi$ takes the coordinate-free tuple $(t, \gamma(t), D\gamma(t), \ldots)$ and gives a coordinate representation as a tuple of the time, the coordinate path function, and as many derivatives of the coordinate path function as are needed. We define the function[23]

$$L_\chi = \mathcal{L} \circ \#_\chi^{-1} \tag{1.6}$$

to be the coordinate representation of the Lagrangian $\mathcal{L}$.

Given a coordinate path $q = \chi \circ \gamma$ the rest of the local description can be computed from it. We introduce a function Γ that does this

$$\Gamma[q](t) = (t, q(t), Dq(t), \ldots) . \tag{1.7}$$

The evaluation of Γ only involves taking derivatives of real-valued functions of real arguments; it does not depend on the particular choice of coordinates. From relations (1.5) and (1.7) we find

$$\Gamma[q] = \Gamma[\chi \circ \gamma] = \#_\chi \circ \mathcal{T}[\gamma]. \tag{1.8}$$

---

[22]We can define $\#_\chi(a, b, c, d, \ldots) = (a, \chi(b), c(\chi), d(\chi), \ldots)$. With this definition:

$$\begin{aligned}\#_\chi(t, \gamma(t), D\gamma(t), D^2\gamma(t), \ldots) &= \big(t, \chi(\gamma(t)), D\gamma(t)(\chi), D^2\gamma(t)(\chi), \ldots\big) \\ &= \big(t, \chi \circ \gamma(t), D(\chi \circ \gamma)(t), D^2(\chi \circ \gamma)(t), \ldots\big) \\ &= \big(t, q(t), Dq(t), D^2q(t), \ldots\big) ,\end{aligned}$$

where we have used the definition of $D^n\gamma$ in footnote 10.

[23]The coordinate function χ is locally invertible, and so is $\#$.

We find a coordinate representation of $\mathcal{L} \circ \mathcal{T}[\gamma]$ using equations (1.6) and (1.8):

$$\mathcal{L} \circ \mathcal{T}[\gamma] = \mathcal{L} \circ \boxplus_{\chi}^{-1} \circ \boxplus_{\chi} \circ \mathcal{T}[\gamma] = L_{\chi} \circ \Gamma[\chi \circ \gamma] = L_{\chi} \circ \Gamma[q]. \quad (1.9)$$

On the left we have the composition of two functions that do not involve coordinates; on the right we have the composition of functions which use the intermediary of a coordinate representation.

The action is

$$\mathcal{S}[\gamma](t_1, t_2) = \int_{t_1}^{t_2} \mathcal{L} \circ \mathcal{T}[\gamma] = \int_{t_1}^{t_2} L_{\chi} \circ \Gamma[q]. \quad (1.10)$$

We can define the coordinate representation of the action as

$$S_{\chi}[q](t_1, t_2) = \int_{t_1}^{t_2} L_{\chi} \circ \Gamma[q]. \quad (1.11)$$

The function S_{χ} takes a coordinate path; the function $\mathcal{S}$ takes a configuration path. We have $\mathcal{S}[\gamma](t_1, t_2) = S_{\chi}[\chi \circ \gamma](t_1, t_2)$. The action for a path is the same in any coordinate system. For Lagrangians that depend only on positions and velocities, the action can also be written

$$S_{\chi}[q](t_1, t_2) = \int_{t_1}^{t_2} L_{\chi}\left(t, q(t), Dq(t)\right) dt. \quad (1.12)$$

When the dependencies are unambiguous, we may leave out the subscripts. For instance, the coordinate system used in the definition of a Lagrangian or an action is usually unambiguous, so the subscript χ will usually be dropped.

1.4 Computing Actions

To illustrate the above ideas, and to introduce their formulation as computer programs, we consider the simplest mechanical system — a free particle moving in three dimensions. Euler and Lagrange discovered that for a free particle the time-integral of the kinetic energy over the particle's actual path is smaller than the same integral along any alternative path between the same points: a free particle moves according to the principle of stationary action, provided we take the Lagrangian to be the kinetic energy. The kinetic energy for a particle of mass m and velocity $\vec{v}$ is $\frac{1}{2}mv^2$, where v is the magnitude of $\vec{v}$. In this case we can choose the generalized coordinates to be the ordinary rectangular coordinates. Let q be the tuple of components of the position with respect to a given rectangular coordinate system, (x, y, z), and let v be the tuple of the velocity components, (v_x, v_y, v_z). Then, following Euler and Lagrange, the Lagrangian for the free particle is[24]

$$L(t, q, v) = \tfrac{1}{2}mv^2. \tag{1.13}$$

We can express this formula as a procedure:

```
(define ((L-free-particle mass) local)
  (let ((v (velocity local)))
    (* 1/2 mass (square v))))
```

The definition indicates that `L-free-particle` is a procedure that takes mass as an argument and returns a procedure of the local tuple that extracts `v` to form the Lagrangian. The procedure `velocity` extracts the generalized velocity from the local tuple.[25]

Suppose we let x denote a coordinate path function that maps time to position components:

$$q(t) = (x(t), y(t), z(t))\,. \tag{1.14}$$

We can make this definition[26]

---

[24]The squared magnitude of the velocity is $\vec{v} \cdot \vec{v}$, the vector dot-product of the velocity with itself. The natural product of a structure of components is the sum of the products of the individual components, so we write simply $v^2 = \vec{v} \cdot \vec{v}$. Whenever there is a natural extension of operators we will do this. It is also natural to extend the arithmetic operations to functions: the combination of two functions of the same type (same domains and ranges) is the function on the same domain that combines the values of the argument functions in the range. For example, if f and g are functions of t, then fg is the function $t \mapsto f(t)g(t)$.

[25]We represent the local tuple as a composite data structure, the components of which are the time, the generalized coordinates, the generalized velocities, and possibly higher derivatives. We do not want to be bothered by the details of packing and unpacking the components into these structures, so we provide utilities for doing this. The constructor `->local` takes the time, the coordinates, and the velocities and returns a data structure representing a local tuple. The selectors `time`, `coordinate`, and `velocity` extract the appropriate pieces from the local structure.

[26]A tuple of coordinate components is made with the procedure `coordinate-tuple`; component `i` of the coordinate tuple `q` is `(ref q i)`. All

```
(define q
  (coordinate-tuple (literal-function 'x)
                    (literal-function 'y)
                    (literal-function 'z)))
```

where `literal-function` makes a function of one argument that has no known properties other than the given symbolic name.[27] The symbol `q` now names a function of one argument that has three literal components. For example, we can evaluate this function for a symbolic time `t` as follows:

```
(print-expression (q 't))
(up (x t) (y t) (z t))
```

The procedure `print-expression` produces a printable form of the expression. The procedure `print-expression` simplifies expressions before printing them.

The derivative of the coordinate path Dq is the function that maps time to velocity components:

$$Dq(t) = (Dx(t), Dy(t), Dz(t)).$$

We can make and use the derivative of a function.[28] For example, we can write:

```
(print-expression ((D q) 't))
(up ((D x) t) ((D y) t) ((D z) t))
```

The function Γ takes a coordinate path and returns a function of time that gives the local tuple $(t, q(t), Dq(t), \ldots)$. We implement this Γ with the procedure `Gamma`. The composition $L \circ \Gamma$ is a function of time that returns the value of the Lagrangian for this point on the path:

---

indexing is zero based. Similarly, a tuple of velocity components is made with `velocity-tuple`; components are selected with `ref`.

[27] In the Scmutils system, arithmetic operators are generic over symbols and expressions as well as numeric values; so arithmetic procedures can work uniformly with numbers or expressions. For example, if we have the procedure `(define (cube x) (* x x x))` we can obtain its value for a number `(cube 2) => 8` or for a literal symbol `(cube 'a) => (* a a a)`.

[28] Derivatives of functions yield functions. For example, `((D cube) 2) => 12` and `((D cube) 'a) => (* 3 (expt a 2))`.

```
(print-expression
  ((compose (L-free-particle 'm) (Gamma q)) 't))
(+ (* 1/2 m (expt ((D x) t) 2))
   (* 1/2 m (expt ((D y) t) 2))
   (* 1/2 m (expt ((D z) t) 2)))
```

The procedure `show-expression` is like `print-expression` except that it puts the simplified expression into traditional infix form and displays the result.[29] Most of the time we will use this method of display, to make the boxed expressions that appear in this book. It also produces the prefix form, but we will usually not show this.[30]

```
(show-expression
 ((compose (L-free-particle 'm) (Gamma q)) 't))
```

$$\boxed{\frac{1}{2}m\,(Dx\,(t))^2 + \frac{1}{2}m\,(Dy\,(t))^2 + \frac{1}{2}m\,(Dz\,(t))^2}$$

According to equation (1.11) we can compute the Lagrangian action from time t_1 to time t_2 as:

```
(define (Lagrangian-action L q t1 t2)
  (definite-integral (compose L (Gamma q)) t1 t2))
```

`Lagrangian-action` takes as arguments a procedure `L` that computes the Lagrangian, a procedure `q` that computes a coordinate path, and starting and ending times `t1` and `t2`. The `definite-integral` used here takes as arguments a function and two limits `t1` and `t2`, and computes the definite integral of the function over the interval from `t1` to `t2`.[31] Notice that the definition of `Lagrangian-action` does not depend on any particular set of coordinates or even the dimension of the configuration space. The method of computing the action from the coordinate representa-

[29] The display is generated with TeX.

[30] For very complicated expressions the prefix notation of Scheme is often better, but simplification is almost always useful. We can separate the functions of simplification and infix display. We will see examples of this later.

[31] Scmutils includes a selection of numerical integration routines. The examples in this section were computed by rational-function extrapolation of Euler-MacLaurin formulas with a relative error tolerance of 10^{-10}.

tion of a Lagrangian and a coordinate path does not depend on the coordinate system.

We can now compute the action for the free particle along a path. For example, consider a particle moving at uniform speed along a straight line $t \mapsto (4t + 7, 3t + 5, 2t + 1)$.[32] We represent the path as a procedure

```
(define (test-path t)
  (coordinate-tuple (+ (* 4 t) 7) (+ (* 3 t) 5) (+ (* 2 t) 1)))
```

For a particle of mass 3, we obtain the action between $t = 0$ and $t = 10$ as

```
(Lagrangian-action (L-free-particle 3)
                   test-path 0 10)
435.
```

Exercise 1.4: Lagrangian actions

For a free particle an appropriate Lagrangian is

$$L(t, x, v) = \frac{1}{2}mv^2.$$

Suppose that x is an actual straight-line path of a free particle, such that $x_a = x(t_a)$ and $x_b = x(t_b)$. Show that the action on the solution path is

$$\frac{m}{2}\frac{(x_b - x_a)^2}{t_b - t_a}.$$

We already know, of course, that the actual path of a free particle is uniform motion in a straight line, and, according to Euler and Lagrange, that the action should be smaller along our test path than along any other nearby path. Let's check this numerically by varying the test path, adding some amount of a test function that is zero at the endpoints $t = t_1$ and $t = t_2$. For example, we could add in a variation equal to $h(t - t_1)(t - t_2)\nu(t)$ where h is a small number and ν is an arbitrary function of the appropriate type:

```
(define ((variation nu t1 t2 h) t)
  (* h (- t t1) (- t t2) (nu t)))
```

[32] Surely for a real physical situation we would have to specify units for these quantities. In this illustration we do not give units.

We can use this to compute the action for a free particle over a path varied from the given path, as a function of h:

```
(define ((varied-free-particle-action mass path nu t1 t2) h)
  (let ((dpath (variation nu t1 t2 h)))
    (Lagrangian-action (L-free-particle mass)
                       (+ path dpath)
                       t1
                       t2)))
```

The action for the varied path, with $\nu(t) = (\sin t, \cos t, t^2)$, and $h = 0.001$ is, as expected, larger than for the test path:

```
((varied-free-particle-action 3.0 test-path
                              (coordinate-tuple sin cos square)
                              0.0 10.0)
 0.001)
436.29121428571153
```

We can numerically compute the value of h for which the action is minimized. We search between, say -2 and 1:[33]

```
(minimize
 (varied-free-particle-action 3.0 test-path
                              (coordinate-tuple sin cos square)
                              0.0 10.0)
 -2.0 1.0)
(-1.5987211554602254e-14 435.0000000000237 5)
```

We find exactly what is expected—that the best value for h is zero, and the minimum value of the action is the action along the straight path.

Finding trajectories that minimize the action

We have used the variational principle to determine if a given trajectory is realizable. We can also use the variational principle to actually find trajectories. Given a set of trajectories that

---

[33] The arguments to `minimize` are: a procedure implementing the univariate function in question, the lower and upper bounds of the region to be searched. Scmutils includes a choice of methods for numerical minimization; the one used here is Brent's algorithm, with an error tolerance of 10^{-5}. The value returned by `minimize` is a list of 3 numbers: the first is the argument at which the minimum occurred, the second is the minimum obtained, and the third is the number of iterations of the minimization algorithm required to obtain the minimum.

are specified by a finite number of parameters, we can search the parameter space looking for the trajectory in the set that best approximates the real trajectory by finding one that extremizes the action. By choosing a good set of approximating functions one can get arbitrarily close to the real trajectory.[34]

One way to make a parametric path that has fixed endpoints is to use a polynomial that goes through the endpoints as well as a number of intermediate points. Variation of the positions of the intermediate points varies the path; the parameters of the varied path are the coordinates of the intermediate positions. The following is a general implementation of such a parametric path maker

```
(define (make-path t0 q0 t1 q1 qs)
  (let ((n (length qs)))
    (let ((ts (linear-interpolants t0 t1 n)))
      (Lagrange-interpolation-function
       (append (list q0) qs (list q1))
       (append (list t0) ts (list t1))))))
```

The procedure `linear-interpolants` produces a list of elements that linearly interpolate the first two arguments. We use this procedure here to specify `ts`, the `n` evenly spaced intermediate times between `t0` and `t1` at which the path will be specified. The parameters being adjusted, `qs`, are the positions at these intermediate times. The procedure `Lagrange-interpolation-function` takes a list of values and a list of times and produces a procedure that computes the Lagrange interpolation polynomial that goes through these points.

Exercise 1.5: Interpolation

a. The procedure `linear-interpolants` can interpolate anything. Use it to find the three linear interpolants between 0 and 4. It can be applied to symbolic inputs: find two linear interpolants of `'x0` and `'x1`. Next find two linear interpolants of `(coordinate-tuple 'x0 'y0)` and `(coordinate-tuple 'x1 'y1)`.

b. Try out the procedure `Lagrange-interpolation-function` by finding the polynomial that goes through the three points $(0, 0)$, $(1, 0)$, $(2, 1)$.

[34] There are lots of good ways to make such a parametric set of approximating trajectories. One could use splines or higher-order interpolating polynomials; one could use Chebyshev polynomials; one could use Fourier components. The choice depends upon the kinds of trajectories one wants to approximate.

Evaluate this polynomial at `x`. This procedure can also interpolate vectors. Try it.

Having specified a parametric path we can construct a parametric action that is just the action computed along the parametric path:

```
(define ((action-on-parametric-path Lagrangian t0 q0 t1 q1) qs)
  (let ((path (make-path t0 q0 t1 q1 qs)))
    (Lagrangian-action Lagrangian path t0 t1)))
```

We can find approximate solution paths by finding parameters that minimize the action. We do this minimization with a canned multidimensional minimization procedure[35]

```
(define (find-path Lagrangian t0 q0 t1 q1 n)
  (let ((initial-qs (linear-interpolants q0 q1 n)))
    (multidimensional-minimize
     (action-on-parametric-path Lagrangian t0 q0 t1 q1)
     initial-qs
     (lambda (converged? qs minimum-value)
       (if converged?
           (make-path t0 q0 t1 q1 qs)
           (error "Minimizer did not converge"))))))
```

The procedure `multidimensional-minimize` takes a procedure (in this case `action-on-parametric-path`) that computes the function to be minimized (in this case the action), an initial guess for the parameters, and a procedure (the `lambda`[36] expression) that is called when the minimizer has found the minimum (or when it gives up). Here we choose the initial path to be a

[35] The minimizer used here is the Nelder-Mead downhill simplex method. As usual with numerical procedures, the interface to the `nelder-mead` procedure is complex, with lots of optional parameters to allow the user to control errors effectively. For this presentation we have specialized `nelder-mead` by wrapping it in the more palatable `multidimensional-minimize`. Unfortunately, you will have to learn to live with complicated numerical procedures someday.

[36] The logician Alonzo Church [5] invented $\boldsymbol{\lambda}$ notation to allow the specification of a function of a named parameter: $\boldsymbol{\lambda} x$[expression in x]. This is read "That function of one argument which is obtained by substituting the argument for x in the indicated expression." Scheme has a special form that implements mathematical $\boldsymbol{\lambda}$-notation: `(lambda (x) ... x ...)`. For example, `(define square (lambda (x) (* x x)))` is the same as `(define (square x) (* x x))`.

straight line between the two endpoints, computed again with `linear-interpolants`.

To illustrate the use of this strategy, we will find trajectories of the harmonic oscillator, with Lagrangian:[37]

$$L(t, q, v) = \tfrac{1}{2}mv^2 - \tfrac{1}{2}kq^2. \tag{1.15}$$

This Lagrangian is implemented by:

```
(define ((L-harmonic m k) local)
  (let ((q (coordinate local))
        (v (velocity local)))
    (- (* 1/2 m (square v)) (* 1/2 k (square q)))))
```

We can find an approximate path taken by the harmonic oscillator for $m = 1$ and $k = 1$ between $q(0) = 1$ and $q(\pi/2) = 0$ as follows:

```
(define q (find-path (L-Harmonic 1.0 1.0) 0. 1. pi/2 0. 3))
```

We know that the trajectories of this harmonic oscillator, for $m = 1$ and $k = 1$, are

$$q(t) = A\cos(t + \varphi) \tag{1.16}$$

where the amplitude A and the phase φ are determined by the initial conditions. For the chosen endpoint conditions the solution is $q(t) = \cos(t)$. The approximate path should be an approximation to cosine over the range from 0 to $\pi/2$. Figure 1.1 shows the error in the polynomial approximation produced by this process. The maximum error in the approximation with three intermediate points is less than 1.7×10^{-4}. We find, as expected that the error in the approximation decreases as the number of intermediate points is increased. For four intermediate points it is about a factor of 15 better.

Exercise 1.6: Solution Process

We can watch the progress of the minimization by modifying the procedure `action-on-parametric-path` procedure to plot the path each time the action is computed. Try this:

---

[37]Don't worry. We know that you don't yet know why this is the right Lagrangian. We will get to this in section 1.6.

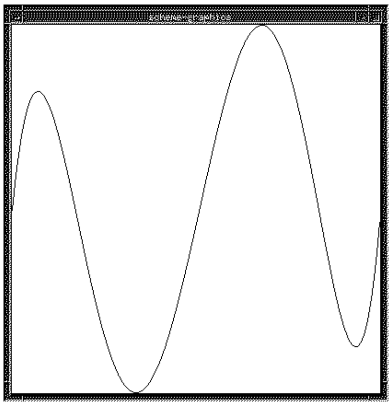

Figure 1.1 The difference between the polynomial approximation with minimum action and the actual trajectory taken by the harmonic oscillator. The abscissa is the time, plotted in the interval $(0, \pi/2)$; the ordinate is the error, plotted in the interval $(-1.65 \times 10^{-4}, 1.68 \times 10^{-4})$.

```
(define win2 (frame 0. pi/2 0. 1.2))

(define ((action-on-parametric-path Lagrangian t0 q0 t1 q1)
         intermediate-qs)
    (let ((path (make-path t0 q0 t1 q1 intermediate-qs)))
      ;; display path
      (graphics-clear win2)
      (plot-function win2 path t0 t1 (/ (- t1 t0) 100))
      ;; compute action
      (Lagrangian-action Lagrangian path t0 t1)))

(find-path (L-harmonic 1. 1.) 0. 1. pi/2 0. 2)
```

Exercise 1.7: Minimizing Action

Suppose we try to obtain a path by minimizing an action for an impossible problem. For example, suppose we have a free particle and we impose endpoint conditions on the velocities as well as the positions that are inconsistent with the particle being free. Does the formalism protect itself from such an unpleasant attack? You may find it illuminating to program it up and see what happens.

1.5 The Euler-Lagrange equations

The principle of stationary action characterizes the realizable paths of systems in configuration space as those for which the action has a stationary value. In elementary calculus, we learn that the critical points of a function are the points where the derivative vanishes. In an analogous way, the paths along which the action is stationary are solutions of a system of differential equations. This system, called the *Euler-Lagrange equations* or just the *Lagrange equations*, is the link that permits us to use the principle of stationary action to compute the motions of mechanical systems, and to relate the variational and Newtonian formulations of mechanics.[38]

Lagrange equations

We will find that if L is a Lagrangian for a system that depends on time, coordinates, and velocities, and if q is a coordinate path for which the action $S[q](t_1, t_2)$ is stationary (with respect to any variation in the path that keeps the endpoints of the path fixed) then

$$D(\partial_2 L \circ \Gamma[q]) - \partial_1 L \circ \Gamma[q] = 0. \tag{1.17}$$

Here L is a real-valued function of a local tuple; $\partial_1 L$ and $\partial_2 L$ denote the partial derivatives of L with respect to its generalized position and generalized velocity arguments.[39] The function $\partial_2 L$ maps a local tuple to a structure whose components are the derivatives of L with respect to each component of the generalized velocity. The function $\Gamma[q]$ maps time to the local tuple: $\Gamma[q](t) = (t, q(t), Dq(t), \ldots)$. Thus the compositions $\partial_1 L \circ \Gamma[q]$ and $\partial_2 L \circ \Gamma[q]$ are functions of one argument, time. Lagrange's equations assert that the derivative of $\partial_2 L \circ \Gamma[q]$ is equal to $\partial_1 L \circ \Gamma[q]$, at any time. Given a Lagrangian, Lagrange's equations form a system of ordinary differential equations that must be satisfied by realizable paths.[40]

---

[38] This result was initially discovered by Euler and later rederived by Lagrange.

[39] The derivative or partial derivative of a function which takes structured arguments is a new function which takes the same number and type of arguments. The range of this new function is itself a structure with the same number of components as the argument with which the derivative is concerned.

[40] Lagrange's equations are traditionally written in the form

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0, \tag{1.18}$$

Varying a path

Suppose that we have a function $f[q]$ that depends on a path q. How does the function vary as the path is varied? Let q be a coordinate path and $q + h\eta$ be a varied path, where the function η is a path-like function that can be added to the path q, and the factor h is a scale factor. We define the *variation* $\delta_\eta f[q]$ of the function f on the path q by

$$\delta_\eta f[q] = \lim_{h \to 0} \left(\frac{f[q + h\eta] - f[q]}{h} \right). \tag{1.20}$$

The variation of f is a linear approximation to the change in the function f for small variations in the path. The variation of f depends on η.

A simple example is the variation of the identity path function: $I[q] = q$. Applying the definition

$$\delta_\eta I[q] = \lim_{h \to 0} \left(\frac{(q + h\eta) - q}{h} \right) = \eta. \tag{1.21}$$

It is traditional to write $\delta I[q]$ simply as δq. Another example is the variation of the path function D that returns the derivative of the path Dq. We have

$$\delta_\eta D[q] = \lim_{h \to 0} \left(\frac{D(q + h\eta) - Dq}{h} \right) = D\eta. \tag{1.22}$$

It is traditional to write $D[q]$ as Dq and $\delta D[q]$ as δDq.

---

or, if we write a separate equation for each component of q, as

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} - \frac{\partial L}{\partial q^i} = 0 \qquad i = 0, \ldots, n-1\,. \tag{1.19}$$

In this way of writing Lagrange's equations the notation does not distinguish between L, which is a real-valued function of three variables $(t, q, \dot{q})$, and $L \circ \Gamma[q]$, which is a real-valued function of one real variable t. If we do not realize this notational pun, the equations don't make sense as written — $\partial L/\partial \dot{q}$ is a function of three variables, so we must regard the arguments $q, \dot{q}$ as functions of t before taking d/dt of the expression. Similarly, $\partial L/\partial q$ is a function of three variables, which we must view as a function of t before setting it equal to $d/dt(\partial L/\partial \dot{q})$. These implicit applications of the chain rule pose no problem in performing hand computations—once you understand what the equations represent.

The variation may be represented in terms of a derivative. Let $g(h) = f[q + h\eta]$. Then

$$\delta_\eta f[q] = \lim_{h \to 0} \left(\frac{g(h) - g(0)}{h} \right) = Dg(0). \tag{1.23}$$

Variations have the following properties. For path-dependent functions f and g and path-independent c:

$$\delta_\eta (f\ g)[q] = \delta_\eta f[q]\ g[q] + f[q]\ \delta_\eta g[q] \tag{1.24}$$

$$\delta_\eta (f + g)[q] = \delta_\eta f[q] + \delta_\eta g[q] \tag{1.25}$$

$$\delta_\eta (cf)[q] = c\ \delta_\eta f[q]. \tag{1.26}$$

Let $h[q] = F \circ g[q]$ with path-independent function F and path-dependent function g, then

$$\delta_\eta h[q] = (DF \circ g[q])\ \delta_\eta g[q]. \tag{1.27}$$

The operators D (differentiation) and δ (variation) commute:

$$D\delta_\eta f[q] = \delta_\eta D(f[q]). \tag{1.28}$$

The statement $\delta_\eta f[q] = 0$ encapsulates the argument that if a path-dependent function f is stationary for a particular path q with respect to small changes in that path then it must be stationary for a subset of those variations that result from adding small multiples of a particular function η to q.

Exercise 1.8: Properties of δ

Show that δ has the properties 1.24-1.28.

Exercise 1.9: Implementation of δ

a. Suppose we have a procedure `f` that implements a path-dependent function: for path `q` and time `t` it has the value `((f q) t)`. The procedure `delta` computes the variation $(\delta_\eta f)[q](t)$ with the value `((((delta eta) f) q) t)`. Complete the definition of `delta`:

```
(define ((((delta eta) f) q) t)
  ...
  )
```

b. Use your `delta` procedure to verify the properties of δ listed in exercise (1.8) for simple functions such as implemented by the procedure `f`:

```
(define ((f q) t)
  ((literal-function 'f*) (q t)))
```

This implements a simple path-dependent function that depends only on the coordinates of the path at each moment.

Derivation of Lagrange's equations:
The action is the integral of the Lagrangian along a path:

$$S[q](t_1, t_2) = \int_{t_1}^{t_2} L \circ \Gamma[q]. \tag{1.29}$$

For a critical path the variation of the action is zero

$$\delta_\eta S[q](t_1, t_2) = 0, \tag{1.30}$$

with respect to variations η that preserve the endpoints $\eta(t_1) = \eta(t_2) = 0$.

The variation of the action is

$$\begin{aligned} \delta_\eta S[q](t_1, t_2) &= \delta_\eta \int_{t_1}^{t_2} (L \circ \Gamma[q]) \\ &= \int_{t_1}^{t_2} \delta_\eta (L \circ \Gamma[q]) \\ &= \int_{t_1}^{t_2} (DL \circ \Gamma[q]) \delta_\eta \Gamma[q] \\ &= \int_{t_1}^{t_2} ((\partial_1 L \circ \Gamma[q]) \delta_\eta q + (\partial_2 L \circ \Gamma[q]) \delta_\eta Dq) \\ &= \int_{t_1}^{t_2} ((\partial_1 L \circ \Gamma[q]) \eta + (\partial_2 L \circ \Gamma[q]) D\eta) \,. \end{aligned} \tag{1.31}$$

Integrating the last term by parts gives

$$\begin{aligned} \delta_\eta S[q](t_1, t_2) = {} & (\partial_2 L \circ \Gamma[q]) \eta |_{t_1}^{t_2} \\ & + \int_{t_1}^{t_2} \{(\partial_1 L \circ \Gamma[q]) - D(\partial_2 L \circ \Gamma[q])\} \, \eta. \end{aligned} \tag{1.32}$$

For variations such that $\eta(t_1) = \eta(t_2) = 0$ the first term vanishes, and the variation of the action is zero if

$$0 = \int_{t_1}^{t_2} \{(\partial_1 L \circ \Gamma[q]) - D(\partial_2 L \circ \Gamma[q])\} \, \eta. \tag{1.33}$$

This must be true for *any* function η that is zero at the endpoints. We retain enough freedom in the choice of the variation so that this forces the factor in the integrand multiplying η to be zero at each point along the path. Suppose this factor were nonzero at some particular time. Then it would have to be nonzero in at least one of its components. But if we choose our η to be a bump that is nonzero only in that component in a neighborhood of that time, and zero everywhere else, then the integral will be nonzero. Thus, the factor in curly brackets is identically zero.[41] We conclude

$$D\left(\partial_2 L \circ \Gamma[q]\right) - \left(\partial_1 L \circ \Gamma[q]\right) = 0, \tag{1.34}$$

which is just what we set out to obtain: Lagrange's equations. So we see that if we restrict the variations to those that keep the endpoints fixed then the critical path satisfies a system of ordinary differential equations at each time.

A path satisfying Lagrange's equations is one for which the action is stationary, and the fact that the action is stationary depends only on the values of L at each point of the path (and at each point on nearby paths), but not on the coordinate system we use to compute these values. So if the system's path satisfies Lagrange's equations in some particular coordinate system, it must satisfy Lagrange's equations in *any* coordinate system. Thus the equations of variational mechanics are derived the same way in any configuration space and any coordinate system.

Example

For an example of calculating with the equations, consider the harmonic oscillator. The Lagrangian is

$$L(t, x, v) = \tfrac{1}{2}mv^2 - \tfrac{1}{2}kx^2.$$

Then

$$\partial_1 L(t, x, v) = -kx \quad \text{and} \quad \partial_2 L(t, x, v) = mv.$$

Now suppose we have a configuration path y. This gives us a local path

$$\Gamma[y](t) = \left(t, y(t), Dy(t)\right).$$

[41] To make this argument more precise requires careful analysis.

So

$$\partial_1 L \circ \Gamma[y] = -ky \quad \text{and} \quad \partial_2 L \circ \Gamma[y] = mDy,$$

and

$$D(\partial_2 L \circ \Gamma[y]) = mD^2 y,$$

so that the Lagrange equations are

$$mD^2 y + ky = 0,$$

which is the equation of motion of the harmonic oscillator.

Exercise 1.10: Calculating Lagrange's Equations

For the following Lagrangians compute Lagrange's equations, showing all of the intermediate steps as we did in the example of the harmonic oscillator.[42]

a. A Lagrangian for a planar pendulum is $L(t, \theta, \dot\theta) = \frac{1}{2} ml^2\dot\theta^2 + mgl\cos\theta$.

b. A Lagrangian for a particle of mass m moving in a two dimensional potential $V(x, y) = (x^2 + y^2)/2 + x^2 y - y^3/3$ is $L(t; x, y; \dot x, \dot y) = \frac{1}{2} m(\dot x^2 + \dot y^2) - V(x, y)$.

c. A Lagrangian for a particle of mass m constrained to move on a sphere of radius R is $L(t; \theta, \varphi; \dot\theta, \dot\varphi) = \frac{1}{2} mR^2(\dot\theta^2 + (\dot\varphi \sin\theta)^2)$, where θ is the colatitude and φ is the longitude on the sphere.

Exercise 1.11: Higher Derivative Lagrangians

Derive Lagrange's equations for Lagrangians that depend on the accelerations. In particular, show that the Lagrange equations for Lagrangians of the form $L(t, q, \dot q, \ddot q)$ with $\ddot q$ terms are:[43]

$$D^2(\partial_3 L \circ \Gamma[q]) - D(\partial_2 L \circ \Gamma[q]) + \partial_1 L \circ \Gamma[q] = 0. \tag{1.35}$$

In general, these equations, first derived by Poisson, will involve the fourth derivative of q. Note that the derivation is completely analogous to the derivation of the Lagrange equations without accelerations; it is

[42] When we write a definition that names the components of the local tuple, we indicate that these are grouped into time, position, and velocity components by separating the groups with semicolons.

[43] In traditional notation these equations read

$$\frac{d^2}{dt^2}\frac{\partial L'}{\partial \ddot q} - \frac{d}{dt}\frac{\partial L'}{\partial \dot q} + \frac{\partial L'}{\partial q} = 0.$$

just longer. What restrictions must we place on the variations so that the critical path satisfies a differential equation?

1.5.1 Computing Lagrange's equations

The procedure for computing Lagrange's equations mirrors the functional expression (1.17), where the procedure `Gamma` implements Γ:[44]

```
(define ((Lagrange-equations Lagrangian) q)
  (let ((local-path (Gamma q)))
    (- (D (compose ((partial 2) Lagrangian) local-path))
       (compose ((partial 1) Lagrangian) local-path))))
```

The argument of `Lagrange-equations` is a procedure that computes a Lagrangian. It returns a procedure that when applied to a path `q`, returns a procedure of one argument (time) that computes the difference of the two sides of Lagrange's equations. These "residual values" will be zero if `q` is a path for which the Lagrangian action is stationary.

Observe that the `Lagrange-equations` procedure, like the Lagrange equations themselves, is valid for *any* generalized coordinate system. When we write programs to investigate particular examples, the procedures that implement the Lagrangian function and the path q will reflect the actual coordinates chosen to represent the system, but we use the same `Lagrange-equations` procedure in each case. This abstraction reflects the important fact that the method of derivation of Lagrange's equations from a Lagrangian is always the same; it is independent of the number of degrees of freedom, the topology of the configuration space, and the particular coordinates used to describe points in the configuration space.

The free particle

Consider again the case of a free particle. The Lagrangian is implemented by the procedure `free-particle-Lagrangian`. Rather than numerically integrating and minimizing the action, as we

---

[44]The `Lagrange-equations` procedure uses the operations `(partial 1)` and `(partial 2)`, which implements the partial derivative operator with respect to the appropriate argument position. This operator can be applied to procedures that describe either scalar-valued or vector-valued functions. In the latter case, the result will be a matrix of partial derivatives.

did above, we can check Lagrange's equations for an arbitrary straight-line path $t \mapsto (at + a_0, bt + b_0, ct + c_0)$

```
(define (test-path t)
  (coordinate-tuple (+ (* 'a t) 'a0)
                    (+ (* 'b t) 'b0)
                    (+ (* 'c t) 'c0)))

(print-expression
 (((Lagrange-equations (L-free-particle 'm))
   test-path)
  't))
(down 0 0 0)
```

That the residuals are zero indicates that the test-path satisfies the Lagrange equations.

Instead of checking the equations for an individual path in three-dimensional space, we can also apply the Lagrange-equations procedure to an arbitrary function:

```
(show-expression
 (((Lagrange-equations (L-free-particle 'm))
   (literal-function 'x))
  't))
(* (((expt D 2) x) t) m)
```

$$\boxed{mD^2x\,(t)}$$

The result is an expression containing the arbitrary time t, and mass m, so it is zero precisely when $D^2x = 0$, which is the expected equation for a free particle.[45]

The harmonic oscillator

Consider the harmonic oscillator again, with Lagrangian (1.15). We know that the motion of a harmonic oscillator is a sinusoid with a given amplitude, frequency and phase:

$$x(t) = a\cos(\omega t + \varphi). \tag{1.36}$$

[45] Observe that the second derivative is indicated as the square of the derivative operator `(expt D 2)`. Arithmetic operations in Scmutils extend over operators as well as functions.

Suppose we have forgotten how the constants in the solution relate to the physical parameters of the oscillator. Let's plug in the proposed solution and look at the residual:

```
(show-expression
 (((Lagrange-equations (L-harmonic 'm 'k))
   (lambda (t) (* 'a (cos (+ (* 'omega t) 'phi)))))
  't))
```

$$\boxed{\cos(\omega t + \varphi)\, a \left(k - m\omega^2\right)}$$

The residual here shows that for nonzero amplitude, the only solutions allowed are ones where $(k - m\omega^2) = 0$, or $\omega = \sqrt{k/m}$. Of course, this is exactly what we would do if calculating by hand.

Exercise 1.12:

Compute Lagrange's equations for the Lagrangians in Exercise 1.10 using the `Lagrange-equations` procedure. Additionally, use the computer to perform each of the steps in the `Lagrange-equations` procedure and show the intermediate results. Relate these steps to the ones you showed in the hand derivation of Exercise 1.10.

Exercise 1.13:

a. Write a procedure to compute the Lagrange equations for Lagrangians that depend upon acceleration, as in exercise 1.11.

b. Use your procedure to compute the Lagrange equations for the Lagrangian

$L(t, x, v, a) = -\frac{1}{2}mxa - \frac{1}{2}kx^2.$

Do you recognize the resulting equation of motion?

c. It is harder, but more fun, to write the general Lagrange equation procedure that takes a Lagrangian of any order, and the order, to produce the required equations of motion.

1.6 How to Find Lagrangians

Lagrange's equations are a system of second-order differential equations. In order to use them to compute the evolution of a mechanical system we must find a suitable Lagrangian for the system. There is no general way to construct a Lagrangian for every system, but there is an important class of systems for which we can identify Lagrangians in a straightforward way in terms of kinetic and potential energy. The key idea is to construct a Lagrangian L such that Lagrange's equations are Newton's equations $\vec{F} = m\vec{a}$.

Suppose our system consists of N particles indexed by α, with mass m_α and vector position $\vec{x}_\alpha(t)$. Suppose further that the forces acting on the particles can be written as the negative gradient of a potential energy V, which is a function of the positions of the particles and possibly time, but which does not depend on the velocities. In other words, the force on particle α is $\vec{F}_\alpha = -\vec{\nabla}_{\vec{x}_\alpha} V$. Then we can rewrite Newton's equations as

$$D(m_\alpha D\vec{x}_\alpha)(t) + \vec{\nabla}_{\vec{x}_\alpha} V(t, \vec{x}_1(t), \ldots, \vec{x}_N(t)) = 0. \tag{1.37}$$

Now suppose we choose as generalized coordinates the rectangular components of the positions of all the particles. The motion of the system is given by the coordinate path x; the coordinates at time t are $x(t) = (\mathbf{x}_1(t), \ldots, \mathbf{x}_N(t))$.[46] Lagrange's equations for the coordinate path x are

$$D\left(\partial_2 L \circ \Gamma[x]\right) - \left(\partial_1 L \circ \Gamma[x]\right) = 0. \tag{1.38}$$

Observe that Newton's equations (1.37) are just the components of the Lagrange equations (1.38) if we choose L to have the properties

$$\begin{aligned} \partial_2 L \circ \Gamma[x](t) &= [m_1 D\mathbf{x}_1(t), \ldots, m_N D\mathbf{x}_N(t)] \\ \partial_1 L \circ \Gamma[x](t) &= [-\nabla_{\mathbf{x}_1} V(t, x(t)), \ldots, -\nabla_{\mathbf{x}_N} V(t, x(t))], \end{aligned} \tag{1.39}$$

where $\nabla_{\mathbf{x}_\alpha} V(t, x(t))$ is the collection of the components of the gradient of V with respect to the coordinates of the particle with

[46]Here $\mathbf{x}_\alpha(t)$ denotes a structure composed of the rectangular components of the vector $\vec{x}_\alpha(t)$. We prefer to group the generalized coordinates in this manner so that we can still conveniently associate them with particular particles. The symbol $x(t)$ refers to the flattened structure of all of the components arranged in sequence.

index α, evaluated at time t and coordinates $x(t)$.[47] We can accomplish this by choosing L so that[48]

$$\partial_2 L(t; \mathbf{x}_1, \ldots, \mathbf{x}_N; \mathbf{v}_1, \ldots, \mathbf{v}_N) = [m_1 \mathbf{v}_1, \ldots, m_N \mathbf{v}_N] \tag{1.40}$$

and

$$\begin{aligned}&\partial_1 L(t; \mathbf{x}_1, \ldots, \mathbf{x}_N; \mathbf{v}_1, \ldots, \mathbf{v}_N) \\ &\quad = [-\nabla_{\mathbf{x}_1} V(t, x), \ldots, -\nabla_{\mathbf{x}_N} V(t, x)].\end{aligned} \tag{1.41}$$

One choice for L that has the required properties (1.40-1.41) is

$$\begin{aligned}L(t, x, v) &= L(t; \mathbf{x}_1, \ldots, \mathbf{x}_N; \mathbf{v}_1, \ldots, \mathbf{v}_N) \\ &= \tfrac{1}{2} \textstyle\sum_\alpha m_\alpha v_\alpha^2 - V(t, x),\end{aligned} \tag{1.42}$$

where v_α is the magnitude of $\mathbf{v}_\alpha$. The first term is the kinetic energy, conventionally denoted T. We see that this choice for the Lagrangian is $L = T - V$, the difference of the kinetic and potential energy.

Hamilton's Principle

Given a system of point particles for which we can identify the force as the (negative) derivative of a potential energy V that is independent of velocity, we have shown that the system evolves along a path that satisfies Lagrange's equations with $L = T - V$. Having identified a Lagrangian for this class of systems, we can restate the principle of stationary action in terms of energies. This statement is known as *Hamilton's Principle*: A point-particle system for which the force is derived from a potential energy that is independent of velocity, evolves along a path q for which the action

$$S[q](t_1, t_2) = \int_{t_1}^{t_2} L \circ \Gamma[q]$$

---

[47]The derivative with respect to a collection of components is the collection of the derivatives with respect to the elements of the collection. A derivative with respect to rectangular components of a vector gives the corresponding rectangular components of the gradient.

[48]As explained in footnote 42, we use the semicolon to separate groups of named components in the arguments.

is stationary with respect to variations of the path q that leave the endpoints fixed, where $L = T - V$ is the difference between kinetic and potential energy.[49]

It might seem that we have reduced Lagrange's equations to nothing more than $\vec{F} = m\vec{a}$, and indeed, the principle is motivated by comparing the two equations for this special class of systems. However, the Lagrangian formulation of the equations of motion has an important advantage over $\vec{F} = m\vec{a}$. Our derivation used the rectangular components $\mathbf{x}_\alpha$ of the positions of the constituent particles for the generalized coordinates, but if the system's path satisfies Lagrange's equations in some particular coordinate system, it must satisfy the equations in *any* coordinate system. Thus we see that $L = T - V$ is suitable as a Lagrangian, with *any* set of generalized coordinates. The equations of variational mechanics are derived the same way in any configuration space and any coordinate system. In contrast, the Newtonian formulation is based on elementary geometry: in order for $D^2\vec{x}(t)$ to be meaningful as an acceleration, $\vec{x}(t)$ must be a vector in physical space. Lagrange's equations have no such restriction on the meaning of the coordinate q. The generalized coordinates can be any parameters which conveniently describe the configurations of the system.

---

[49] Hamilton formulated the fundamental variational principle, which C. G. J. Jacobi later named "Hamilton's principle" in 1834-35, for systems where $L = T - V$, with T a quadratic form in the generalized velocities, and L independent of time. For systems subject to generic, nonstationary constraints Hamilton's principle was investigated in 1848 by M. V. Ostrogradsky, and that is why in the Russian literature it is often called the Hamilton-Ostrogradsky principle.

William Rowan Hamilton (1805–1865) was a brilliant 19th-century mathematician. His early work on geometric optics (based on Fermat's principle) was so impressive that he was elected to the post of Professor of Astronomy at Trinity College and Royal Astronomer of Ireland while he was still an undergraduate. He produced two monumental works of 19th-century mathematics. His discovery of quaternions revitalized abstract algebra and sparked the development of vector techniques in physics. His 1835 memoir "On a General Method in Dynamics" put variational mechanics on a firm footing, finally giving substance to Maupertuis's vaguely stated Principle of Least Action of 100 years before. Hamilton also wrote poetry and carried on an extensive correspondence with Wordsworth, who advised him to put his energy into writing mathematics rather than poetry.

In addition to the formulation of the fundamental variational principle, Hamilton also stressed the analogy between geometric optics and mechanics, and stressed the importance of the momentum variables (which were earlier introduced by Lagrange and Cauchy), leading to the "canonical" form of mechanics, which we discuss in chapter 3.

Constant acceleration

Consider a particle of mass m in a uniform gravitational field with acceleration g. The potential energy is $V = mgh$ where h is the height of the particle. The kinetic energy is just $T = \frac{1}{2}mv^2$. A Lagrangian for the system is $T-V$. In rectangular coordinates, with y measuring the vertical position and x measuring the horizontal position, the Lagrangian is $L(t; x, y; v_x, v_y) = \frac{1}{2}m\left(v_x^2 + v_y^2\right) - mgy$. We have

```
(define ((L-uniform-acceleration m g) local)
  (let ((q (coordinate local))
        (v (velocity local)))
    (let ((y (ref q 1)))
      (- (* 1/2 m (square v)) (* m g y)))))

(show-expression
 (((Lagrange-equations
    (L-uniform-acceleration 'm 'g))
   (coordinate-tuple (literal-function 'x)
                     (literal-function 'y)))
  't))
(down (* m (((expt D 2) x) t))
      (+ (* g m) (* m (((expt D 2) y) t))))
```

$$\begin{bmatrix} mD^2x(t) \\ gm + mD^2y(t) \end{bmatrix}$$

This equation describes unaccelerated motion in the horizontal direction $mD^2x = 0$ and constant acceleration in the vertical direction $mD^2y = -gm$.

Central force field

Consider planar motion of a particle of mass m in a central force field, with an arbitrary potential energy $V(r)$, depending only on the radius. The kinetic energy is $T = \frac{1}{2}mv^2$. A Lagrangian for the system is $L = T - V$. We will derive the Lagrange equations for this system in both rectangular coordinates and polar coordinates.

In rectangular coordinates (x, y) the Lagrangian is

$$L(t; x, y; v_x, v_y) = \tfrac{1}{2}m(v_x^2 + v_y^2) - V(\sqrt{x^2 + y^2}). \qquad (1.43)$$

As a procedure:

```
(define ((L-central-rectangular m V) local)
  (let ((q (coordinate local))
        (v (velocity local)))
    (- (* 1/2 m (square v))
       (V (sqrt (square q))))))
```

The Lagrange equations are

```
(show-expression
 (((Lagrange-equations
    (L-central-rectangular 'm (literal-function 'V)))
   (coordinate-tuple (literal-function 'x)
                     (literal-function 'y)))
  't))
```

$$\boxed{\begin{bmatrix} mD^2x(t) + \dfrac{DV\left(\sqrt{(y(t))^2 + (x(t))^2}\right)x(t)}{\sqrt{(y(t))^2 + (x(t))^2}} \\ mD^2y(t) + \dfrac{DV\left(\sqrt{(x(t))^2 + (y(t))^2}\right)y(t)}{\sqrt{(x(t))^2 + (y(t))^2}} \end{bmatrix}}$$

We can rewrite these Lagrange equations as:

$$mD^2x = -\frac{x}{r}DV(r) \tag{1.44}$$

$$mD^2y = -\frac{y}{r}DV(r), \tag{1.45}$$

where $r = \sqrt{x^2 + y^2}$. We can interpret these as follows. The particle is subject to a radially directed force with magnitude $-DV(r)$. Newton's equations equate the force with the product of the mass and the acceleration. The two Lagrange equations are just the rectangular components of Newton's equations.

Now we describe this system in polar coordinates r and φ such that $x = r\cos\varphi$ and $y = r\sin\varphi$. The kinetic energy is $T = \frac{1}{2}m(v_x^2 + v_y^2)$. The components of the rectangular velocities can be found by substituting coordinate paths into the transformation equations, differentiating, and abstracting to arbitrary velocities. With $x = r\cos\varphi$ and $y = r\sin\varphi$ we obtain

$$\begin{aligned} v_x &= \dot{r}\cos\varphi - r\dot{\varphi}\sin\varphi \\ v_y &= \dot{r}\sin\varphi + r\dot{\varphi}\cos\varphi. \end{aligned} \tag{1.46}$$

So the kinetic energy is[50]

$$T(t; r, \varphi; \dot{r}, \dot{\varphi}) = \tfrac{1}{2}m(\dot{r}^2 + r^2\dot{\varphi}^2), \tag{1.47}$$

and the Lagrangian is

$$L(t; r, \varphi; \dot{r}, \dot{\varphi}) = \tfrac{1}{2}m(\dot{r}^2 + r^2\dot{\varphi}^2) - V(r). \tag{1.48}$$

We express this Lagrangian as follows:

```
(define ((L-central-polar m V) local)
  (let ((q (coordinate local))
        (qdot (velocity local)))
    (let ((r (ref q 0)) (phi (ref q 1))
          (rdot (ref qdot 0)) (phidot (ref qdot 1)))
      (- (* 1/2 m
            (+ (square rdot)
               (square (* r phidot))) )
         (V r)))))
```

Lagrange's equations are:

```
(show-expression
 (((Lagrange-equations
    (L-central-polar 'm (literal-function 'V)))
   (coordinate-tuple (literal-function 'r)
                     (literal-function 'phi)))
  't))
```

$$\begin{bmatrix} mD^2r(t) - mr(t)(D\varphi(t))^2 + DV(r(t)) \\ \\ 2mDr(t)\,r(t)\,D\varphi(t) + mD^2\varphi(t)\,(r(t))^2 \end{bmatrix}$$

We can interpret the first equation as expressing that the product of the mass and the radial acceleration is the sum of the force due to the potential and the centrifugal force. The second equation can be interpreted as saying that the derivative of the angular momentum $mr^2D\varphi$ is zero; so angular momentum is conserved.[51]

Note that we used the same `Lagrange-equations` procedure for the derivation in both coordinate systems. Coordinate repre-

---

[50] Alternatively, we can recognize that the components of the velocity are $\dot{r}$ in the radial direction and $r\dot{\varphi}$ in the direction perpendicular to the radius. So $v^2 = \dot{r}^2 + r^2\dot{\varphi}^2$.

[51] We will talk much more about angular momentum later.

sentations of the Lagrangian are different for different coordinate systems. The Lagrange equations in different coordinate systems look different. Yet, the same method is used to derive the Lagrange equations in any coordinate system.

Exercise 1.14:

Check that the Lagrange equations for central force motion in polar coordinates and the Lagrange equations in rectangular coordinates are equivalent. Determine the relationship among the second derivatives by substituting paths into the transformation equations and computing derivatives, then substitute these relations into the equations of motion.

1.6.1 Coordinate Transformations

The motion of a system is independent of the coordinates we use to describe it. This coordinate-free nature of the motion is apparent in the action principle. The action depends only on the value of the Lagrangian along the path and not on the particular coordinates used in the representation of the Lagrangian. We can use this property to find a Lagrangian in one coordinate system in terms of a Lagrangian in another coordinate system.

Suppose we have a mechanical system whose motion is described by a Lagrangian $L(t, q, v)$, and a coordinate transformation F such that $q = F(t, q')$. One way to find a Lagrangian expressed in the primed coordinates that describes the same system is to require that the value of the Lagrangian along the path be independent of the coordinate system:

$$L' \circ \Gamma[q'] = L \circ \Gamma[q]. \tag{1.49}$$

Let C be the function that maps local tuples in the primed coordinate system to local tuples in the unprimed coordinate system

$$C \circ \Gamma[q'] = \Gamma[q]. \tag{1.50}$$

Then if we choose

$$L' = L \circ C, \tag{1.51}$$

we have

$$L' \circ \Gamma[q'] = L \circ C \circ \Gamma[q'] = L \circ \Gamma[q], \tag{1.52}$$

and requirement (1.49) is satisfied.

The function C must map local tuples in one coordinate system to local tuples in another coordinates system in a way that satisfies the "kinematic" requirement (1.50). The coordinate transformation specifies the relationship of the coordinates $q = F(t, q')$. To complete the specification of C we need to determine how the generalized velocities transform. Let q and q' be the same configuration path expressed in different coordinate systems. Substituting these paths into the coordinate transformation and computing the derivative we find

$$Dq(t) = \partial_0 F(t, q'(t)) + \partial_1 F(t, q'(t)) Dq'(t). \tag{1.53}$$

Through any point there is always a path of any given velocity, so we may generalize, and conclude that along corresponding coordinate paths the generalized velocities satisfy

$$v = \partial_0 F(t, q') + \partial_1 F(t, q')v'. \tag{1.54}$$

We can use this to define the function C that takes a local tuple in the primed system to a local tuple in the unprimed system

$$\begin{aligned}(t,\ q,\ v,\ \ldots) &= C(t,\ q',\ v',\ \ldots) \\ &= (t,\ F(t,q'),\ \partial_0 F(t,q') + \partial_1 F(t,q')v',\ \ldots).\end{aligned} \tag{1.55}$$

If needed, rules for higher derivative components of the local tuple can be determined in a similar fashion.

So if we take the Lagrangian L' to be

$$L' = L \circ C \tag{1.56}$$

then the action has a value that is independent of the coordinate system used to compute it. The configuration path of stationary action does not depend on which coordinate system is used to describe the path. The Lagrange equations which are derived from these Lagrangians will in general look very different from one another, but they must be equivalent.

Exercise 1.15:

Show by direct calculation that the Lagrange equations for L' are satisfied if the Lagrange equations for L are satisfied.

Given a coordinate transformation F, we can use equation (1.55) to find the function C, which transforms local tuples. The procedure `F->C` implements this

```
(define ((F->C F) local)
  (let ((t (time local))
        (q (coordinate local))
        (v (velocity local)))
    (->local t
             (F t q)
             (+ (((partial 0) F) t q)
                (* (((partial 1) F) t q) v)))))
```

As an illustration, consider the transformation from polar to rectangular coordinates: $x = r\cos\varphi$ and $y = r\sin\varphi$, with the following implementation:

```
(define (p->r t polar-tuple)
  (let ((r (ref polar-tuple 0))
        (phi (ref polar-tuple 1)))
    (let ((x (* r (cos phi)))
          (y (* r (sin phi))))
      (coordinate-tuple x y))))
```

In terms of the polar coordinates and the rate of change of the polar coordinates, the rate of change of the rectangular components are:

```
(show-expression
 (velocity
  ((F->C p->r)
   (->local 't
    (coordinate-tuple 'r 'phi)
    (velocity-tuple 'rdot 'phidot)))))
```

$$\boxed{\begin{pmatrix} -\dot{\varphi} r \sin(\varphi) + \dot{r}\cos(\varphi) \\ \dot{\varphi} r \cos(\varphi) + \dot{r}\sin(\varphi) \end{pmatrix}}$$

We can use `F->C` to find the Lagrangian for central force motion in polar coordinates from the Lagrangian in rectangular components, using equation (1.51),

```
(define (L-central-polar m V)
  (compose (L-central-rectangular m V) (F->C p->r)))

(show-expression
  ((L-central-polar 'm (literal-function 'V))
   (->local 't (coordinate-tuple 'r 'phi)
               (velocity-tuple 'rdot 'phidot))))
```

$$\boxed{\frac{1}{2}m\dot{\varphi}^2r^2 + \frac{1}{2}m\dot{r}^2 - V(r)}$$

The result is the same as Lagrangian (1.48).

Local Functions from Path Functions

An essential step in the derivation of the local tuple transformation function C from the coordinate transformation F was the deduction of the relationship between the velocities in the two coordinate systems. We did this by inserting coordinate paths into the coordinate transformation function F, differentiating, and then generalizing the results on the path to arbitrary velocities at a moment. The last step is an example of a more general problem of deducing a local tuple function from a path function. Given a function f of a local tuple a corresponding path-dependent function $\bar{f}[q]$ is $\bar{f}[q] = f \circ \Gamma[q]$. Given $\bar{f}$ how can we reconstitute f? We can reconstruct a local tuple function from a path function by finding a path that has the given local description and then passing this path to the path function.

Suppose we have a function of a local description that depends on a finite number of components of the local description. This function has the same value on all paths for which those components are the same. Two paths that have the same local description up to the nth derivative are said to osculate with order n contact. For example, a path and the truncated power series representation of the path up to order n have order n contact; if fewer than n derivatives are needed by a local tuple function, the path and the truncated power series representation are equivalent. Let O be a function that generates an osculating path with the given local components. So $O(t, q, v, \ldots)(t) = q$, $D(O(t, q, v, \ldots))(t) = v$, and in general

$$(t, q, v, \ldots) = \Gamma[O(t, q, v, \ldots)](t). \tag{1.57}$$

The number of components of the local description that are required is finite, but unspecified. One way of constructing O is through the truncated power series

$$O(t, q, v, a, \ldots)(t') = q + v(t' - t) + \tfrac{1}{2}a(t' - t)^2 + \cdots, \qquad (1.58)$$

where the number of terms is the same as the number of components of the local description that are specified.

To reconstruct f from $\bar{f}$ we need to compute the value of f given some number of components of the local description. The local tuple can be used to construct an osculating path, and the value of f for that local tuple is obtained by passing this osculating path to $\bar{f}$:

$$\bar{f}[O(t, q, v, \ldots)](t) = f \circ \Gamma[O(t, q, v, \ldots)](t) = f(t, q, v, \ldots). \quad (1.59)$$

Let $\bar{\Gamma}$ be the function that takes a path function and returns the corresponding local function:

$$f = \bar{\Gamma}(\bar{f}). \qquad (1.60)$$

From equation (1.59) we see that

$$\bar{\Gamma}(\bar{f})(t, q, v, \ldots) = \bar{f}[O(t, q, v, \ldots)](t). \qquad (1.61)$$

The procedure `Gamma-bar` implements the function $\bar{\Gamma}$ that reconstitutes a path-dependent function into a local function:

```
(define ((Gamma-bar f) local)
  ((f (osculating-path local)) (time local)))
```

The procedure `osculating-path` takes a number of local components and returns a path with these components; it is implemented as a power series.

We can use `Gamma-bar` to make an alternate implementation of the procedure `F->C`:

```
(define (F->C F)
  (Gamma-bar
   (lambda (q)
     (Gamma
      (lambda (t) (F t (q t)))))))
```

We specify the local tuple transformation for a given coordinate transformation by defining a path function that makes a local tuple path for a transformed path and then making this path function into the corresponding local tuple function. Notice that in this definition of `F->C` we do not explicitly calculate any derivatives. The calculation that led up to the state transformation (1.55) is not needed.

Exercise 1.16: Path Functions and State Functions

The local function f is the same as the local function $\bar{\Gamma}(\bar{f})$ where $\bar{f}[q] = f \circ \Gamma[q]$. On the other hand, the path function $\bar{f}[q]$, and the path function $\bar{\Gamma}(\bar{f}) \circ \Gamma[q]$, are not generally the same. Explain. Give examples where they are the same and where they are not the same. Write programs to illustrate the behavior.

Exercise 1.17: Central Force Motion

Find Lagrangians for central force motion in three dimensions in rectangular coordinates and spherical coordinates. First, find the Lagrangians analytically, then check the results with the computer, generalizing the programs presented to three dimensions.

1.6.2 Systems with Rigid Constraints

We have found that $L = T - V$ is a suitable Lagrangian for a system of point particles subject to forces derived from a potential. Extended bodies can sometimes be conveniently idealized as absolutely rigid. We will find that $L = T - V$, expressed in irredundant coordinates, is also a suitable Lagrangian for these systems. We will first illustrate the method and then provide a justification.

Lagrangians for rigidly constrained systems

The system is presumed to be made of N mass points in ordinary 3-dimensional space. The first step is to choose a convenient set of non-redundant generalized coordinates q and redescribe the system in terms of these. Non-redundant coordinates are coordinates for which all the coordinate constraints are built into the functions f_α. The relationship expressing the rectangular coordinates in terms of the generalized coordinates is

$$\mathbf{x}_\alpha = f_\alpha(t, q). \tag{1.62}$$

We deduce the relationship of the generalized velocities v to the velocities of the constituent particles $\mathbf{v}_\alpha$ by inserting path functions

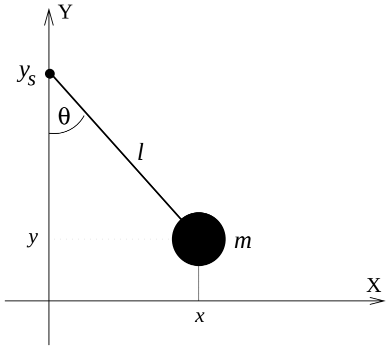

Figure 1.2 The driven pendulum

into equation (1.62), differentiating, and abstracting to arbitrary velocities. We find

$$\mathbf{v}_\alpha = \partial_0 f_\alpha(t, q) + \partial_1 f_\alpha(t, q)v. \tag{1.63}$$

The kinetic energy, which is the sum of the kinetic energies of the constituent particles, can now be expressed in terms of the generalized coordinates and velocities:

$$\begin{aligned} T(t, q, v) &= \sum_\alpha \tfrac{1}{2} m_\alpha \mathbf{v}_\alpha^2 \\ &= \sum_\alpha \tfrac{1}{2} m_\alpha (\partial_0 f_\alpha(t, q) + \partial_1 f_\alpha(t, q)v)^2 \end{aligned} \tag{1.64}$$

Similarly, we use equation (1.62) to reexpress the potential energy in terms of the generalized coordinates.

We take the Lagrangian to be the difference of the kinetic and potential energies: $L = T - V$, where the kinetic and potential energies are expressed in terms of the generalized coordinates and velocities.

A pendulum driven at the pivot

Consider a pendulum (see figure 1.2), of length l, and mass m supported by a pivot that is driven in the vertical direction by a given function of time y_s.

The dimension of the configuration space for this system is one; we choose θ, shown in figure 1.2, as the generalized coordinate.

The position of the bob is given, in rectangular coordinates, by

$$x = l \sin\theta \qquad y = y_s(t) - l\cos\theta.$$

The velocities are

$$v_x = l\dot\theta\cos\theta \qquad v_y = Dy_s(t) + l\dot\theta\sin\theta,$$

obtained by differentiating along a path and abstracting to velocities at the moment.

The kinetic energy is

$$\begin{aligned} T(t,\theta,\dot\theta) &= \tfrac{1}{2}m(v_x^2+v_y^2) \\ &= \tfrac{1}{2}m\left(l^2\dot\theta^2 + (Dy_s(t))^2 + 2l\ Dy_s(t)\ \dot\theta\ \sin\theta\right). \end{aligned}$$

and the potential energy is

$$V(t,\theta,\dot\theta) = gmy = gm\left(y_s(t) - l\cos\theta\right).$$

A Lagrangian is $L = T - V$.

The Lagrangian is expressed as

```
(define ((T-pend m l g ys) local)
  (let ((t (time local))
        (theta (coordinate local))
        (thetadot (velocity local)))
    (let ((ysdot (D ys)))
      (* 1/2 m
         (+ (square (* l thetadot))
            (square (ysdot t))
            (* 2 (ysdot t) l (sin theta) thetadot))))))

(define ((V-pend m l g ys) local)
  (let ((t (time local))
        (theta (coordinate local)))
    (* m g (- (ys t) (* l (cos theta))))))

(define L-pend (- T-pend V-pend))
```

Lagrange's equation for this system is

```
(show-expression
 (((Lagrange-equations
     (L-pend 'm 'l 'g (literal-function 'y_s)))
   (literal-function 'theta))
  't))
```

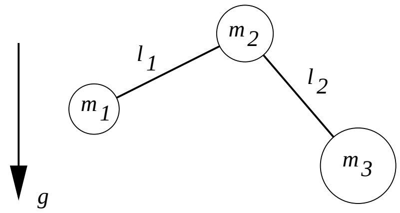

Figure 1.3 A two-bar linkage

$$\boxed{D^2\theta\,(t)\, l^2 m + D^2 y_s\,(t) \sin\left(\theta\,(t)\right) lm + \sin\left(\theta\,(t)\right) glm}$$

Exercise 1.18:

Show that the Lagrangians in Exercise 1.10 represent the systems indicated.

Exercise 1.19: Bead on a Helical Wire

A bead of mass m is constrained to move on a frictionless helical wire. The helix is oriented so that its axis is horizontal. The diameter of the helix is d and its pitch (turns per unit length) is h. The system is in a uniform gravitational field with acceleration g. Formulate a Lagrangian that describes the system and find the Lagrange equations of motion.

Exercise 1.20: Bead on a Triaxial Surface

A bead of mass m moves without friction on a triaxial ellipsoidal surface. In rectangular coordinates the surface satisfies

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1, \tag{1.65}$$

for some constants a, b, and c. Identify suitable generalized coordinates, formulate a Lagrangian, and find Lagrange's equations.

Exercise 1.21: A Two-bar Linkage

The two-bar linkage shown in figure 1.3 is constrained to move in the plane. It is composed of three small massive bodies interconnected by two massless rigid rods in a uniform gravitational field with acceleration g. The rods are pinned to the central body by a hinge that allows the linkage to fold. Let assume that the system is arranged so that the hinge is completely free: the members can go through all configurations without collision. Formulate a Lagrangian that describes the system and find the Lagrange equations of motion. Use the computer to do this, because the equations are rather big.

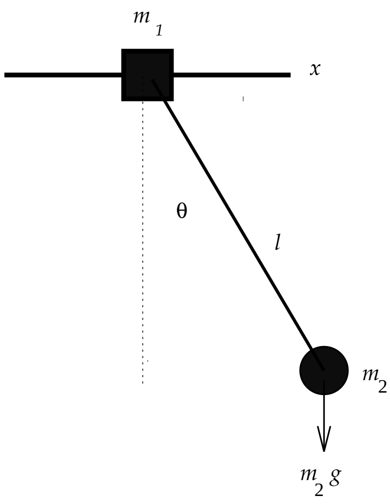

Figure 1.4 The sliding pendulum

Exercise 1.22: Sliding Pendulum

Consider a pendulum of length l attached to a support that is free to move horizontally. (See Figure 1.4.) Let the mass of the support be m_1 and the mass of the pendulum be m_2. Formulate a Lagrangian and derive Lagrange's equations for this system.

Why it works

In this section we show that a suitable Lagrangian for rigidly constrained systems is $L = T - V$. We do this by requiring that the Lagrange equations are equivalent to the Newtonian vectorial dynamics with vector constraint forces.[52]

We consider a system of particles. The particle with index α has mass m_α and position $\vec{x}_\alpha$. There may be a very large number of these particles, or just a few. Some of the positions may also be given functions of time, such as the position of the pivot of

[52] We will simply accept the Newtonian procedure for systems with rigid constraints and find Lagrangians which are equivalent. Of course, actual bodies are never truly rigid, so we may wonder what detailed approximations have to be made to treat them as truly rigid. For instance, a more satisfying approach would be to replace the rigid distance constraints by very stiff springs. We could then immediately write the Lagrangian as $L = T - V$, and we should be able to *derive* the Newtonian procedure for systems with rigid constraints as an approximation. However, this is too complicated to do at this stage, so for the time being we accept the Newtonian idealization.

a driven pendulum. There are rigid position constraints among some of the particles; we assume all of these constraints are of the form

$$(\vec{x}_\alpha - \vec{x}_\beta) \cdot (\vec{x}_\alpha - \vec{x}_\beta) = l^2_{\alpha\beta}, \tag{1.66}$$

the distance between particles α and β is $l_{\alpha\beta}$.

The Newtonian equation of motion for particle α is

$$m_\alpha D^2 \vec{x}_\alpha = -\vec{\nabla}_{\vec{x}_\alpha} V + \sum_{\{\beta | \beta \leftrightarrow \alpha\}} \vec{F}^c_{\alpha\beta}, \tag{1.67}$$

where in the summation β ranges over only those particle indices for which there are rigid constraints with the particle indexed by α; we use the notation $\beta \leftrightarrow \alpha$ for the relation that there is a rigid constraint between the indicated particles.

The mass times the acceleration of particle α is equal to the sum of the potential forces and the constraint forces. The potential forces are derived as the negative gradient of the potential energy, and may depend on the positions of the other particles and the time. The constraint forces $\vec{F}_{\alpha\beta}$ are the vector constraint forces associated with the rigid constraint between particle α and particle β. The force of constraint is directed along the line between the particles, so we may write

$$\vec{F}_{\alpha\beta} = \frac{\vec{x}_\beta - \vec{x}_\alpha}{l_{\alpha\beta}} F_{\alpha\beta} \tag{1.68}$$

where $F_{\alpha\beta}$ is the scalar magnitude of the tension in the constraint. Note that $\vec{F}_{\alpha\beta} = -\vec{F}_{\beta\alpha}$. In general, the scalar constraint forces change as the system evolves.

Formally, we can reproduce Newton's equations with the Lagrangian[53]

[53] This Lagrangian is purely formal and does not represent a model of the constraint forces. In particular, note that the constraint terms do not look like a potential of constraint with a minimum when the constraint is exactly satisfied. Rather, the constraint terms in the Lagrangian are zero when the constraint is satisfied, and can be either positive or negative depending on the whether the distance between the particles is larger or smaller than the constraint distance.

$$L(t;x,F;\dot{x},\dot{F}) = \sum_\alpha \tfrac{1}{2} m_\alpha \dot{\mathbf{x}}_\alpha^2 - V(t,x) + \sum_{\{\alpha,\beta|\alpha<\beta,\alpha\leftrightarrow\beta\}} \frac{F_{\alpha\beta}}{2l_{\alpha\beta}} \left[(\mathbf{x}_\beta - \mathbf{x}_\alpha)^2 - l_{\alpha\beta}^2\right] \quad (1.69)$$

where the constraint forces are being treated as additional generalized coordinates. Here x is a structure composed of all of the rectangular components $\mathbf{x}_\alpha$ of all of the $\vec{x}_\alpha$, $\dot{x}$ is a structure composed of all the rectangular components $\dot{\mathbf{x}}_\alpha$ of all of the velocity vectors $\vec{v}_\alpha$, and F is a structure composed of all of the $F_{\alpha\beta}$. The velocity of F does not appear in the Lagrangian, and F itself only appears linearly. So the Lagrange equations associated with F are

$$(\mathbf{x}_\beta - \mathbf{x}_\alpha)^2 - l_{\alpha\beta}^2 = 0 \quad (1.70)$$

but this is just a restatement of the constraints. The Lagrange equations for the particle coordinates are Newton's equations (1.67)

$$mD^2\mathbf{x}_\alpha = -\nabla_{\mathbf{x}_\alpha} V(t,x) + \sum_{\{\beta|\alpha\leftrightarrow\beta\}} F_{\alpha\beta} \frac{\mathbf{x}_\beta - \mathbf{x}_\alpha}{l_{\alpha\beta}}. \quad (1.71)$$

Now that we have a suitable Lagrangian, we can use the fact that Lagrangians can be reexpressed in any generalized coordinates to find a simpler Lagrangian. Let q be generalized coordinates which specify the degrees of freedom of the system without redundancy. Let F be the scalar constraint forces, and c be the distances between particles for which constraints are specified

$$c_{\alpha\beta} = \left[(\vec{x}_\beta - \vec{x}_\alpha) \cdot (\vec{x}_\beta - \vec{x}_\alpha)\right]^{1/2}. \quad (1.72)$$

Then we choose as our new coordinates the set of components of q, c, and F. There exist functions f_α that give the coordinates of the constituent particles in terms of q and c:

$$\mathbf{x}_\alpha = f_\alpha(t,q,c). \quad (1.73)$$

To reexpress the Lagrangian in terms of q and c we need to find $\mathbf{v}_\alpha$ in terms of the generalized velocities $\dot{q}$ and $\dot{c}$: we do this by differentiating f_α along a path and abstracting to arbitrary velocities (see Section 1.6.1):

$$\mathbf{v}_\alpha = \partial_0 f_\alpha(t, q, c) + \partial_1 f_\alpha(t, q, c)\ \dot{q} + \partial_2 f_\alpha(t, q, c)\ \dot{c}. \tag{1.74}$$

Substituting these into Lagrangian (1.69) we find

$$\begin{aligned} &L'(t; q, c, F; \dot{q}, \dot{c}, \dot{F}) \\ &\quad = \sum_\alpha \tfrac{1}{2} m_\alpha \left(\partial_0 f_\alpha(t, q, c) + \partial_1 f_\alpha(t, q, c)\ \dot{q} + \partial_2 f_\alpha(t, q, c)\ \dot{c}\right)^2 \\ &\qquad - V(t, f(t, q, c)) + \sum_{\{\alpha,\beta \mid \alpha<\beta, \alpha\leftrightarrow\beta\}} \frac{F_{\alpha\beta}}{2 l_{\alpha\beta}} \left[c^2_{\alpha\beta} - l^2_{\alpha\beta}\right]. \end{aligned} \tag{1.75}$$

The Lagrange equations are derived by the usual procedure. Rather than write out all the gory details, let's think about how it will go. The Lagrange equations associated with F just restate the constraints:

$$0 = c^2_{\alpha\beta}(t) - l^2_{\alpha\beta} \tag{1.76}$$

and consequently we know that along a solution path $c(t) = l$, and $Dc(t) = D^2 c(t) = 0$. We can use this result to simplify the Lagrange equations associated with q and F. The Lagrange equations associated with q are the same as if they were derived from the Lagrangian[54]

$$\begin{aligned} L''(t, q, \dot{q}) = &\sum_\alpha \tfrac{1}{2} m_\alpha \left(\partial_0 f_\alpha(t, q, l) + \partial_1 f_\alpha(t, q, l)\ \dot{q}\right)^2 \\ &- V(t, f(t, q, l)), \end{aligned} \tag{1.77}$$

but this is exactly $T - V$ where T and V are computed from the generalized coordinates q, with fixed constraints. Notice that the constraint forces do not appear in the Lagrange equations for q because in the Lagrange equations they are multiplied by a term that is identically zero on the solution paths. So the Lagrange

[54] Consider a function g of, say, three arguments, and let g_0 be a function of two arguments satisfying $g_0(x, y) = g(x, y, 0)$. Then $(\partial_0 g_0)(x, y) = (\partial_0 g)(x, y, 0)$. The substitution of a value in an argument commutes with the taking of the partial derivative with respect to a different argument. In deriving the Lagrange equations for q we can set $c = l$ and $\dot{c} = 0$ in the Lagrangian, but we cannot do this in deriving the Lagrange equations associated with c, because we have to take derivatives with respect to those arguments.

equations for $T - V$ with irredundant generalized coordinates q and fixed constraints is equivalent to the Newtonian procedure with vector constraint forces.

The Lagrange equations for c can be used to find the constraint forces. The Lagrange equations are a big mess so we will not show them explicitly, but in general they are equations in D^2c, Dc, and c which will depend upon q, Dq, and F. The dependence on F is linear, so we can solve for F in terms of the solution path q and Dq, with $c = l$ and $Dc = D^2c = 0$. If we are not interested in the constraint forces, we can abandon the full Lagrangian (1.75) in favor of Lagrangian (1.77) which is equivalent as far as the evolution of the generalized coordinates q are concerned.

More generally

The same derivation goes through even if the lengths $l_{\alpha\beta}$ specified in the interparticle distance constraints are a function of time. It can also be generalized to allow distance constraints to time-dependent positions, by making some of the positions of particles $\vec{x}_\beta$ explicit functions of time rather than dynamical variables.

In fact the argument can be generalized for any constraint that depends only on the time and coordinates. We express the constraint as

$$\varphi(t, x) = 0, \tag{1.78}$$

where x is again the structure of all the rectangular components $\mathbf{x}_\alpha$ of all the $\vec{x}_\alpha$. The constraints are enforced by the addition of extra constraint forces to each of Newton's equations:

$$m_\alpha D^2\vec{x}_\alpha = -\vec{\nabla}_{\vec{x}_\alpha} V + \sum_\alpha \vec{F}^c_\alpha, \tag{1.79}$$

Formally, we can reproduce these equations with the Lagrangian

$$L(t; x, \lambda; \dot{x}, \dot{\lambda}) = \sum_\alpha \tfrac{1}{2} m_\alpha \dot{\mathbf{x}}^2_\alpha - V(t, x) + \lambda\varphi(t, x). \tag{1.80}$$

Note again that the term added to the Lagrangian here is not a potential energy for the constraint. As before, the Lagrange equations associated with λ are just a restatement of the constraints, and the Lagrange equations for the particle coordinates are:

$$m_\alpha D^2\vec{x}_\alpha = -\vec{\nabla}_{\vec{x}_\alpha} V + \lambda\partial_{1,\alpha}\varphi(t, x). \tag{1.81}$$

For equations (1.81) to be the same as equations (1.79) we must identify $\lambda \partial_{1,\alpha}\varphi(t,x)$ with the forces of constraint on particle α. Notice that these forces of constraint are proportional to the normal to the constraint surface at each instant and thus do no work for motions that obey the constraint.[55]

Indeed, in the special derivation for rigid distance constraints we can identify

$$\lambda\varphi(t,x) = \sum_{\{\alpha,\beta|\alpha<\beta,\alpha\leftrightarrow\beta\}} \frac{F_{\alpha\beta}}{2l_{\alpha\beta}}\left[(\mathbf{x}_\beta - \mathbf{x}_\alpha)^2 - l_{\alpha\beta}^2\right]. \tag{1.82}$$

The forces of constraint are then identified

$$\lambda\partial_{1,\alpha}\varphi(t,x) = \sum_{\{\beta|\alpha\leftrightarrow\beta\}} F_{\alpha\beta}\frac{\mathbf{x}_\beta - \mathbf{x}_\alpha}{l_{\alpha\beta}}. \tag{1.83}$$

The derivation must then proceed to transform from the redundant coordinates, x to the irredundant coordinates q with constant constraint coordinates, $c = \varphi(t,x)$, as above. The coordinate λ will not appear in the Lagrange equations for q because on solution paths they will be multiplied by a factor that is identically zero.

Thus the Lagrangian $L = T - V$ is equivalent to Newton's vectorial equations for any system of point masses moving under potential forces whether or not there are rigid constraints among the coordinates. The potential and the constraints can be explicitly time dependent.

Exercise 1.23: The Dumbell

In this exercise we will recapitulate the derivation of the Lagrangian for constrained systems for a particular simple system.

Consider two massive particles in the plane constrained by a massless rigid rod to remain a distance l apart, as in figure 1.5. There are apparently four degrees of freedom for two massive particles in the plane, but the rigid rod reduces this number to three, as we can uniquely spec-

---

[55] The force of constraint is normal to the constraint surface. This is equivalent to the fact that the projection of the residual of Newton's equations without constraint forces,

$$m_\alpha D^2\vec{x}_\alpha + \vec{\nabla}_{\vec{x}_\alpha}V,$$

onto the constraint surface is zero. The latter is sometimes referred to as d'Alembert's Principle.

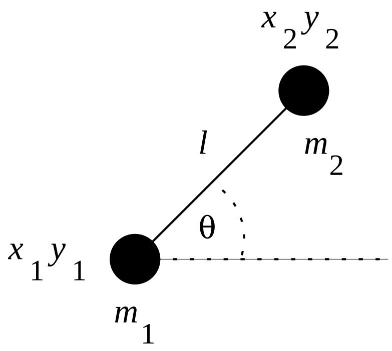

Figure 1.5 A rigid rod of length l constrains two massive particles in a plane.

ify the configuration using as generalized coordinates the coordinates of one particle, say x_1, x_2 and the angle θ that gives the orientation of one of the particles relative to the other, because we have the constraint $(x_2 - x_1)^2 + (y_2 - y_1)^2 = l^2$.

a. Write Newton's equations of the balance of forces for the four rectangular coordinates of the two particles, given that the scalar tension in the rod is F.

b. Write the formal Lagrangian

$$L(t; x_1, y_1, x_2, y_2, F; \dot{x}_1, \dot{y}_1, \dot{x}_2, \dot{y}_2, \dot{F})$$

such that Lagrange's equations will yield the Newton's equations that you derived in part **a**.

c. Make a change of coordinates to a coordinate system with coordinates x_1, y_1, θ, c, F such that c is the distance between the masses. Write the Lagrangian in these coordinates, and write the Lagrange equations.

d. You may deduce from one of these equations that $c = l$. From this fact we get that $Dc = 0$ and $D^2c = 0$. Substitute these into the Lagrange equations you just computed to get equations of motion for x_1, y_1, θ.

e. Make a Lagrangian ($= T - V$) for the system described with the irredundant generalized coordinates x_1, y_1, θ and compute the Lagrange equations from this Lagrangian. They should be the same equations as you derived for the same coordinates from part **d**.

Exercise 1.24:

Fill in the details. Show that the Lagrange equations for Lagrangian (1.77) are the same as the Lagrange equations for Lagrangian (1.75) with the substitution $c(t) = l$, $Dc(t) = D^2c(t) = 0$.

Exercise 1.25: Constraint Forces

a. Find the tension in an undriven planar pendulum.

b. A particle of mass m slides off a horizontal cylinder of radius R in a uniform gravitational field with acceleration g. If the particle starts at the top with zero initial speed, with what angular velocity does the particle leave the cylinder?

1.6.3 Constraints as Coordinate Transformations

The derivation of a Lagrangian for a constrained system involves steps that are analogous to the steps in the derivation of a coordinate transformation. For a constrained system one specifies generalized coordinates and from the definition deduces how the velocities of the constituent particles depend on the coordinates and the generalized velocities. The Lagrangian can then be written in terms of the kinetic and potential energies of the constituent particles. Alternatively, to carry out a coordinate transformation one specifies the relationship of the coordinates and from this specification deduces how the generalized velocities are related, by exactly the same process. These are really two applications of the same process. Our deduction that $L = T - V$ is a suitable Lagrangian for a constrained systems was in fact based on a coordinate transformation from a set of coordinates subject to constraints to a set of irredundant coordinates plus constraint coordinates that are constant. We can develop Lagrangians for constrained systems in such a way that this connection to coordinate transformations is explicit.

Let $x = (\mathbf{x}_1, \ldots, \mathbf{x}_N)$ be the collection of rectangular coordinate components of the constituent particles, and $v = (\mathbf{v}_1, \ldots, \mathbf{v}_N)$ be the corresponding collection of rectangular velocity components of the constituent particles. The Lagrangian

$$L_f(t, x, v) = \sum_\alpha \tfrac{1}{2} m_\alpha v_\alpha^2 - V(x) \tag{1.84}$$

is the difference of kinetic and potential energies of the constituent particles. This is a suitable Lagrangian for a set of unconstrained free particles with potential energy V.

Let q be a set of irredundant generalized coordinates. These are related to $\mathbf{x}_\alpha$, the coordinates of the constituent particles, by

$$\mathbf{x}_\alpha = f_\alpha(t, q), \tag{1.85}$$

as before. The constraints among the constituent particles are taken into account in the definition of the f_α. Here we view this as a coordinate transformation. What is unusual about this as a coordinate transformation is that the dimension of x is not the same as the dimension of q. From this coordinate transformation we can find the local tuple transformation function.

A Lagrangian for the constrained system can be obtained from the Lagrangian for the unconstrained system by composing it with the local tuple transformation function from constrained coordinates to unconstrained coordinates. The constraints enter only in the transformation.

To illustrate this we will find a Lagrangian for the driven pendulum. The $T - V$ Lagrangian for a free particle of mass m in a vertical plane subject to a gravitational potential with acceleration g is

$$L_f(t; x, y; v_x, v_y) = \tfrac{1}{2}m(v_x^2 + v_y^2) - mgy, \tag{1.86}$$

where y measures the vertical height of the mass point. As a program

```
(define ((Lf m g) local)
  (let ((q (coordinate local))
        (v (velocity local)))
    (let ((h (ref q 1)))
      (- (* 1/2 m (square v)) (* m g h)))))
```

The coordinate transformation from generalized coordinate θ to rectangular coordinates is $x = l \sin\theta$, $y = y_s(t) - l\cos\theta$, where l is the length of the pendulum and y_s gives the height of the support as a function of time. It is interesting that the drive enters only through the specification of the constraints. As a program

```
(define ((dp-coordinates l y_s) t theta)
  (let ((x (* l (sin theta)))
        (y (- (y_s t) (* l (cos theta)))))
    (coordinate-tuple x y)))
```

Using `F->C` we can deduce the local tuple transformation and define the Lagrangian for the driven pendulum by composition:

```
(define (L-pend m l g y_s)
  (compose (Lf m g)
           (F->C (dp-coordinates l y_s))))
```

The Lagrangian is

```
(show-expression
 ((L-pend 'm 'l 'g (literal-function 'y_s))
  (->local 't 'theta 'thetadot)))
```

$$\boxed{glm\cos(\theta) - gmy_s(t) + \frac{1}{2}l^2m\dot\theta^2 + lm\dot\theta Dy_s(t)\sin(\theta) + \frac{1}{2}m\left(Dy_s(t)\right)^2}$$

This is the same as the Lagrangian found in section 1.6.2.

We have found a very interesting decomposition of the Lagrangian for constrained systems. One part consists of the difference of the kinetic and potential energy of the constituents. The other part describes the constraints which are specific to the configuration of a particular system. It is tempting to say that the first part describes the physics and the second the kinematics of the configuration space.

1.6.4 The Lagrangian is not unique

Lagrangians are not in a one to one relationship with physical systems—many Lagrangians can be used to describe the same physical system. In this section we will show that the addition to the Lagrangian of a "total time derivative of a function of the coordinates and time" does not change the paths of stationary action or the equations of motion deduced from the action principle.

Total Time Derivatives

Let's first explain what we mean by a "total time derivative." Let $F(t, q)$ depend solely on t and q. Then the time derivative of F along a path q is

$$\begin{aligned} D(F \circ \Gamma[q]) &= (DF \circ \Gamma[q])D\Gamma[q] \\ &= (\partial_0 F \circ \Gamma[q]) + (\partial_1 F \circ \Gamma[q])Dq \\ &= (\partial_0 F + (\partial_1 F)\dot Q) \circ \Gamma[q], \end{aligned} \tag{1.87}$$

where $\dot Q$ is a selector function: $c = \dot Q(a, b, c)$, or $Dq = \dot Q \circ \Gamma[q]$. The function

$$D_t F = \partial_0 F + (\partial_1 F)\dot Q \tag{1.88}$$

is the total time derivative of F; it is a function of three arguments: the time, the generalized coordinates, and the generalized velocities. Composed with a path it is the time derivative of the composition of the function F with the same path:

$$D_t F \circ \Gamma[q] = D(F \circ \Gamma[q]). \tag{1.89}$$

For more general functions F of some number of local components, the total time derivative $D_t F$ is defined by

$$D_t F = \bar{\Gamma}(\bar{G}), \qquad \text{with} \qquad \bar{G}[q] = (D(F \circ \Gamma[q])). \tag{1.90}$$

An explicit formula for computing the total time derivative $D_t F$ of the function F is

$$\begin{aligned} D_t F(t, q, v, a, \ldots) = \partial_0 F(t, q, v, a, \ldots) \\ + \partial_1 F(t, q, v, a, \ldots)\, v \\ + \partial_2 F(t, q, v, a, \ldots)\, a \\ + \cdots, \end{aligned} \tag{1.91}$$

where we take as many terms as needed to exhaust the arguments of F.

The implementation of the total time derivative as a program follows the definition (1.90). Given a procedure `F` implementing a local function and a path `q` we can construct a new procedure `(compose F (Gamma q))`. The procedure `G-bar` implements the derivative of this function of time. We then abstract this off the path with `Gamma-bar` to give the total time derivative.

```
(define (Dt F)
  (define (G-bar q)
    (D (compose F (Gamma q))))
  (Gamma-bar G-bar))
```

Exercise 1.26: Properties of D_t

The total time derivative $D_t F$ is not the derivative of the function F. Nevertheless, the total time derivative shares many properties with the derivative. For local functions F and G, and number c, demonstrate that D_t has the following properties:

a. $D_t(F + G) = D_t F + D_t G$

b. $D_t(cF) = c D_t F$

c. $D_t(FG) = F D_t G + (D_t F) G$

d. $D_t(F \circ G) = (DF \circ G) D_t G$.

Lagrangians

Consider two Lagrangians L and L' that differ by the addition of a total time derivative of a function F that depends only on the time and the coordinates

$$L' = L + D_t F. \tag{1.92}$$

The corresponding action integral is

$$\begin{aligned} S'[q](t_1, t_2) &= \int_{t_1}^{t_2} L' \circ \Gamma[q] \\ &= \int_{t_1}^{t_2} (L + D_t F) \circ \Gamma[q] \\ &= \int_{t_1}^{t_2} L \circ \Gamma[q] + \int_{t_1}^{t_2} D(F \circ \Gamma[q]) \\ &= S[q](t_1, t_2) + (F \circ \Gamma[q])|_{t_1}^{t_2}. \end{aligned} \tag{1.93}$$

The variational principle states that the action integral along a realizable trajectory is stationary with respect to variations of the trajectory that leave the configuration at the endpoints fixed. The action integrals $S[q](t_1, t_2)$ and $S'[q](t_1, t_2)$ differ by a term

$$(F \circ \Gamma[q])|_{t_1}^{t_2} = F(t_2, q(t_2)) - F(t_1, q(t_1)) \tag{1.94}$$

that depends only on the coordinates and time at the endpoints and these are not allowed to vary. Thus, if $S[q](t_1, t_2)$ is stationary for a path, then $S'[q](t_1, t_2)$ will also be stationary. So either Lagrangian can be used to distinguish the realizable paths.

The addition of a total time derivative to a Lagrangian does not affect whether the action is critical for a given path. Therefore, the Lagrange equations satisfied by the critical path must be unchanged by the addition of a total time derivative to the Lagrangian. The equations of motion are not changed if terms are added to the Lagrangian that when composed with a path comprise the time derivative of the composition of a function of the coordinates and time with the path.

Exercise 1.27: Adding Total Time Derivatives to Lagrangians

Let $F(t, q)$ be a function of t and q only, with total time derivative

$$D_t F = \partial_0 F + \partial_q F \dot{Q}. \tag{1.95}$$

Show explicitly that the Lagrange equations for $D_t F$ are identically zero, and thus that the addition of $D_t F$ to a Lagrangian does not affect the Lagrange equations.

The driven pendulum provides a nice illustration of adding total time derivative to Lagrangians. The equation of motion for the driven pendulum (see section 1.6.2),

$$ml^2 D^2\theta(t) + ml(g + D^2 y_s(t)) \sin\theta(t) = 0, \tag{1.96}$$

has an interesting and suggestive interpretation: it is the same as the equation of motion of an undriven pendulum, except that the acceleration of gravity g is augmented by the acceleration of the pivot $D^2 y_s$. This intuitive interpretation was not apparent in the Lagrangian derived as the difference of the kinetic and potential energies in Section (1.6.2). However, we can write an alternate Lagrangian that has the same equations of motion that is as easy to interpret as the equation of motion:

$$L'(t, \theta, \dot{\theta}) = \frac{1}{2}ml^2\dot{\theta}^2 + ml(g + D^2 y_s(t)) \cos\theta. \tag{1.97}$$

With this Lagrangian it is apparent that the effect of the accelerating pivot is to modify the acceleration of gravity. Note, however, that it is not the difference of the kinetic and potential energies. Let's compare the two Lagrangians for the driven pendulum. The difference $\Delta L = L - L'$ is

$$\begin{aligned}\Delta L(t, \theta, \dot{\theta}) = {} & \frac{1}{2}m(Dy_s(t))^2 + mlDy_s(t)\dot{\theta}\sin\theta \\ & - gmy_s(t) - mlD^2 y_s(t)\cos\theta.\end{aligned} \tag{1.98}$$

The two terms in ΔL which do not depend on either θ or $\dot{\theta}$ do not affect the equations of motion. The remaining two terms are the total time derivative of the function $F(t, \theta) = -mlDy_s(t)\cos\theta$, which does not depend on $\dot{\theta}$. The addition of such terms to a Lagrangian does not affect the equations of motion.

Identification of Total Time Derivatives

How can one tell if a given function, when composed with a path, is the total time derivative of another function of the coordinates and time? Let $G(t, q, v)$ be a candidate function. By comparing with equation (1.88), we see that G must be linear in the generalized velocities

$$G(t, q, v) = G_1(t, q)\ v + G_2(t, q) \tag{1.99}$$

where neither G_1 nor G_2 depend on the generalized velocities. Because $G_1 = \partial_1 F$ and $G_2 = \partial_0 F$, we must have

$$\partial_0 G_1 = \partial_1 G_2. \tag{1.100}$$

Furthermore, because $G_1 = \partial_1 F$, then

$$\partial_1 G_1 = \partial_1 \partial_1 F \tag{1.101}$$

must be symmetric: If there is more than one degree of freedom these partials are actually structures of partial derivatives with respect to each coordinate. The partial derivatives with respect to two different coordinates must be the same independent of the order of the differentiation. Note that we have not shown that these conditions are sufficient for determining that a function is a total time derivative, only that they are necessary.

Exercise 1.28: Identifying Total Time Derivatives

For each of the following functions, either show that it is not a total time derivative or produce a function from which it may be derived.

a. $G(t, x, v_x) = m v_x$

b. $G(t, x, v_x) = m v_x \cos t$

c. $G(t, x, v_x) = v_x \cos t - x \sin t$

d. $G(t, x, v_x) = v_x \cos t + x \sin t$

e. $G(t; x, y; v_x, v_y) = 2(x v_x + y v_y) \cos t - (x^2 + y^2) \sin t$

f. $G(t; x, y; v_x, v_y) = 2(x v_x + y v_y) \cos t - (x^2 + y^2) \sin t + y^3 v_x + x v_y$

1.7 Lagrange Equations at a Moment

Realizable paths satisfy the Lagrange equations; the Lagrange equations relate the path and its derivatives at each moment. For a realizable path q, the Lagrange equations relate the coordinates $q(t)$, the velocities $Dq(t)$, and the accelerations $D^2 q(t)$ at the moment t.[56] The Lagrange equations can be rewritten as a relation among the components of the local description of the path at a moment.

Let $\bar{\mathsf{E}}[L]$ be the path-dependent function that produces the residuals on the path of the Lagrange equations for the Lagrangian L:

$$\bar{\mathsf{E}}[L][q] = D(\partial_2 L \circ \Gamma[q]) - \partial_1 L \circ \Gamma[q]. \tag{1.102}$$

Realizable paths q satisfy the Lagrange equations

$$\bar{\mathsf{E}}[L][q] = 0. \tag{1.103}$$

The path-dependent Lagrange equations can be converted to local Lagrange equations using $\bar{\Gamma}$

$$\mathsf{E}[L] = \bar{\Gamma}(\bar{\mathsf{E}}[L]). \tag{1.104}$$

The operator E is called the *Euler-Lagrange operator*. In terms of this operator the Lagrange equations are

$$\mathsf{E}[L] \circ \Gamma[q] = 0. \tag{1.105}$$

Applying the definition (1.61) of $\bar{\Gamma}$

$$\begin{aligned}
\mathsf{E}[L](t, q, v, \ldots) &= \bar{\Gamma}(\bar{\mathsf{E}}[L])(t, q, v, \ldots) \\
&= D(\partial_2 L \circ \Gamma[O(t, q, v, \ldots)]) \\
&\quad - \partial_1 L \circ \Gamma[O(t, q, v, \ldots)] \\
&= (D_t(\partial_2 L))(t, q, v, \ldots) - \partial_1 L(t, q, v, \ldots) \\
&= (D_t \partial_2 L - \partial_1 L)(t, q, v, \ldots).
\end{aligned} \tag{1.106}$$

So the Euler-Lagrange operator is explicitly

$$\mathsf{E}[L] = D_t \partial_2 L - \partial_1 L. \tag{1.107}$$

The procedure `Euler-Lagrange-operator` implements E

```
(define (Euler-Lagrange-operator L)
  (- (Dt ((partial 2) L)) ((partial 1) L))) .
```

[56] There may be higher derivatives of the path that participate in the Lagrange equations if the Lagrangian depends on higher derivatives than the velocities.

For example, applied to the Lagrangian for the harmonic oscillator,

```
(show-expression
 ((Euler-Lagrange-operator
   (L-harmonic 'm 'k))
  (->local 't 'x 'v 'a)))
(+ (* a m) (* k x))
```

Notice that the components of the local description are individually specified. The Lagrange-equations for the harmonic oscillator are:[57]

```
(show-expression
 ((compose
   (Euler-Lagrange-operator (L-harmonic 'm 'k))
   (Gamma (literal-function 'x) 4))
  't))
(+ (* k (x t)) (* m (((expt D 2) x) t)))
```

Exercise 1.29: Properties of E

Let F and G be two Lagrangian-like functions of a local tuple, C be a local tuple transformation function, and c a constant. Demonstrate the following properties:

a. $\mathsf{E}[F + G] = \mathsf{E}[F] + \mathsf{E}[G]$

b. $\mathsf{E}[cF] = c\mathsf{E}[F]$

c. $\mathsf{E}[FG] = \mathsf{E}[F]G + F\mathsf{E}[G] + (D_t F)\partial_2 G + \partial_2 F(D_t G)$

d. $\mathsf{E}[F \circ C] = D_t(DF \circ C)\partial_2 C + DF \circ C\mathsf{E}[C]$

The operator E is linear, but it does not satisfy the Leibnitz product rule.

1.8 Evolution of Dynamical State

Lagrange's equations are ordinary differential equations that the path must satisfy. They can be used to test if a proposed path is a realizable path of the system. However, we can also use them to develop a path, starting with initial conditions.

The *state* of a system is defined to be the information that must be specified for the subsequent evolution to be determined.

---

[57]Notice that `Gamma` has one more argument than it usually has. This argument gives the length of the local description returned. The default length is 3, returning the local tuple up to the velocities.

Remember our juggler: he or she must throw the pin in a certain way for it to execute the desired motion. The juggler has control of the initial position and orientation of the pin, and the initial velocity and spin of the pin. Our experience with juggling and similar systems suggests that the initial configuration and the rate of change of the configuration are sufficient to determine the subsequent motion. Other systems may require higher derivatives of the configuration.

For Lagrangians that are written in terms of a set of generalized coordinates and velocities we have shown that Lagrange's equations are second-order ordinary differential equations. If the differential equations can be solved for the highest-order derivatives and if the differential equations satisfy appropriate conditions[58] then there is a unique solution to the initial-value problem: given values of the solution and the lower derivatives of the solution at a particular moment there is a unique solution function. Given non-redundant coordinates the Lagrange equations satisfy these conditions.[59] Thus a trajectory is determined by the generalized coordinates and the generalized velocities at any time. This is the information required to specify the dynamical state.

A local description of a path consists of the path and all of its derivatives at a moment. The complete local description of a path can be reconstructed from an initial segment of the local description, given a prescription for computing higher derivatives of the path in terms of lower derivatives. The state of the system is specified by that initial segment of the local description from which the rest of the local description can be deduced. The full local description gives us the path near that moment. Actually, all we need is a rule for computing the next higher derivative; we can get all the rest from this. Assume that the state of a system

---

[58] For example, the Lipschitz condition is that the rate of change of the derivative is bounded by a constant in an open set around each point of the trajectory. See [12] for a good treatment of the Lipschitz condition.

[59] If the coordinates are redundant we cannot, in general solve for the highest-order derivative. However, since we can transform to non-redundant coordinates, and since we can solve the initial-value problem in the non-redundant coordinates, and since we can construct the redundant coordinates from the non-redundant coordinates, we can in general solve the initial-value problem for redundant coordinates. The only hitch is that we may not specify arbitrary initial conditions: the initial conditions must be consistent with the constraints.

is given by the local tuple (t, q, v). If we are given a prescription for computing the acceleration $a = A(t, q, v)$, then

$$D^2 q = A \circ \Gamma[q], \tag{1.108}$$

and we have as a consequence

$$D^3 q = D(A \circ \Gamma[q]) = D_t A \circ \Gamma[q], \tag{1.109}$$

and so on. So the higher derivative components of the local tuple are given by functions $D_t A$, $D_t^2 A$, ... Each of these functions depends on lower derivative components of the local description. All we need to deduce the path from the state is a function that gives the next higher derivative component of the local description from the state. We use the Lagrange equations to find this function.

First, we expand the Lagrange equations

$$\partial_1 L \circ \Gamma[q] = D(\partial_2 L \circ \Gamma[q])$$

so that the second derivative appears explicitly

$$\begin{aligned}&\partial_1 L \circ \Gamma[q] \\ &\quad = \partial_0 \partial_2 L \circ \Gamma[q] + (\partial_1 \partial_2 L \circ \Gamma[q])\, Dq + (\partial_2 \partial_2 L \circ \Gamma[q])\, D^2 q.\end{aligned}$$

Solving this system for $D^2 q$ one obtains the generalized acceleration along a solution path q

$$\begin{aligned}&D^2 q = \\ &\quad [\partial_2 \partial_2 L \circ \Gamma[q]]^{-1} [\partial_1 L \circ \Gamma[q] - (\partial_1 \partial_2 L \circ \Gamma[q])\, Dq - \partial_0 \partial_2 L \circ \Gamma[q]]\end{aligned}$$

where $[\partial_2 \partial_2 L \circ \Gamma]^{-1}$ is the inverse of the Hessian matrix. The function that gives the acceleration is

$$A = [(\partial_2 \partial_2 L)]^{-1} \left[\partial_1 L - \partial_0 \partial_2 L - (\partial_1 \partial_2 L)\dot{Q}\right], \tag{1.110}$$

where $\dot{Q}$ is the velocity component selector.

That initial segment of the local description that specifies the state is called the local state tuple, or, more simply, the state tuple.

We can express the function that gives the acceleration as a function of the local state tuple as the following procedure. It takes a procedure that computes the Lagrangian, and returns a procedure that takes a local state tuple as its argument and returns the acceleration.[60]

```
(define (Lagrangian->acceleration L)
  (let ((P ((partial 2) L))
        (F ((partial 1) L)))
    (/ (- F
          (+ ((partial 0) P)
             (* ((partial 1) P) velocity)))
       ((partial 2) P))))
```

Once we have a way of computing the acceleration from the coordinates and the velocities, we can give a prescription for computing the derivative of the local state as a function of the local state. For the state $(t, q(t), Dq(t))$ at the moment t the derivative of the state is $(1, Dq(t), D^2q(t)) = (1, Dq(t), A(t, q(t), Dq(t)))$. This gives an alternate form of the Lagrange equations, expressed as a first-order system.

```
(define ((Lagrange-equations-1 L) q v)
  (let ((local-path (qv->local-path q v)))
    (- (D local-path)
       (compose (local-state-derivative L)
local-path))))

(define ((local-state-derivative L) local)
  (->local 1
   (velocity local)
   ((Lagrangian->acceleration L) local)))

(define ((qv->local-path q v) t)
  (->local t (q t) (v t)))
```

For example, we can find the first-order form of the equations of motion of a two-dimensional harmonic oscillator:

```
(show-expression
 (((Lagrange-equations-1 (L-harmonic 'm 'k))
   (coordinate-tuple (literal-function 'x)
                     (literal-function 'y))
   (velocity-tuple (literal-function 'v_x)
                   (literal-function 'v_y)))
  't))
```

[60] In Scmutils division by a matrix is interpreted as multiplication on the left by the inverse matrix.

$$\begin{pmatrix} 0 \\ \begin{pmatrix} Dx(t) - v_x(t) \\ Dy(t) - v_y(t) \end{pmatrix} \\ \begin{pmatrix} \dfrac{kx(t)}{m} + Dv_x(t) \\ \dfrac{ky(t)}{m} + Dv_y(t) \end{pmatrix} \end{pmatrix}$$

The zero in first element of the structure of the Lagrange equations residuals is just the tautology that time advances uniformly: that the time function is just the identity, so its derivative is 1 and the residual is zero. The equations in the second element constrain the velocity path to be the derivative of the coordinate path. The equations in the third element give the rate of change of the velocity in terms of the applied forces.

Numerical Integration

The numerical solution of a differential equation is often formulated in terms of an equivalent system of first order differential equations, as shown in Figure 1.6. Our numerical integrators want unstructured state, rather than states with coordinate components and velocity components grouped separately. They also want the derivative of that state to be a flat structure as well. In the following procedure, which takes a Lagrangian and produces a state derivative procedure, the local tuple is constructed from the integrator state by the procedure `istate->local` and an unstructured state is constructed from local components by the procedure `->istate`.

```
(define (Lagrangian->state-derivative L)
  (let ((acceleration (Lagrangian->acceleration L)))
    (lambda (istate)
      (let ((local (istate->local istate)))
        (->istate 1
                  (velocity local)
                  (acceleration local))))))
```

The state derivative produced by this procedure can be used by a package that numerically integrates systems of first order differential equations.

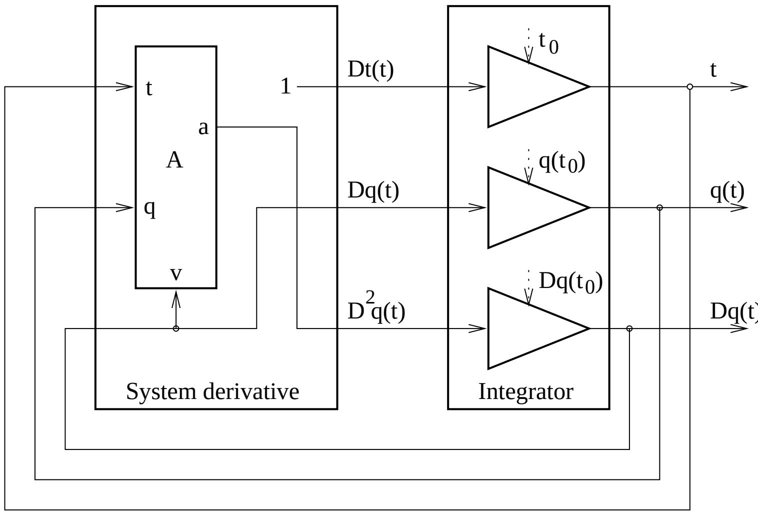

Figure 1.6 The input to the system derivative is the state. The function A gives the acceleration as a function of the local components that determine the state. The output of the system derivative is the derivative of the state. The integrator takes the derivative of the state as its input and produces the integrated state, starting at the initial conditions. Notice how the second-order system is put into first-order form by the routing of the $Dq(t)$ components in the system derivative.

Let's illustrate this process with the driven pendulum described above. In this system, a periodic drive is interesting. We choose $y_s(t) = a \cos \omega t$.

```
(define ((periodic-drive amplitude frequency phase) t)
  (* amplitude (cos (+ (* frequency t) phase))))

(define (L-periodically-driven-pendulum m l g a omega)
  (let ((ys (periodic-drive a omega 0)))
    (L-pend m l g ys)))
```

Lagrange's equation for this system is:

```
(show-expression
 (((Lagrange-equations
    (L-periodically-driven-pendulum 'm 'l 'g 'a 'omega))
   (literal-function 'theta))
  't))
```

$$\boxed{D^2\theta(t)\, l^2 m - \cos(\omega t)\sin(\theta(t))\, a l m \omega^2 + \sin(\theta(t))\, g l m}$$

The state derivative for the periodically driven pendulum is

```
(show-expression
 ((Lagrangian->state-derivative
   (L-periodically-driven-pendulum 'm 'l 'g 'a 'omega))
  (->istate 't 'theta 'thetadot)))
```

$$\boxed{\begin{pmatrix} 1 \\ \dot{\theta} \\ \dfrac{\sin(\theta)\left(\cos(\omega t)\, a\omega^2 - g\right)}{l} \end{pmatrix}}$$

To get the parametric version of the state derivative, we write

```
(define (pend-sysder m l g a omega)
  (Lagrangian->state-derivative
    (L-periodically-driven-pendulum m l g a omega)))
```

Once we have a state derivative we may integrate it numerically by a suitable method and study the evolution of the system, for various initial conditions. Although the `pend-sysder` procedure could be used for a numerical integration experiment it would be exceedingly slow because the mathematical operations are general enough to manipulate such monstrosities as matrices full of symbolic expressions. To make this useful for numerical computation we compile it with the procedure `compile-parametric`. The arguments are the number of state variables (we include the time) and the system derivative:

```
(define pend-sysder-compiled
  (compile-parametric 3 pend-sysder))
```

For example, to investigate the trajectory of a driven pendulum we write a program built around the procedure `ode-advancer`[61]

[61] The Scmutils system provides a stable of numerical integration routines that can be accessed through this interface. These include quality-controlled Runge-Kutta (QCRK4) and Bulirsch-Stoer. The default integrator, which is being set up here, is QCRK4.

that takes a procedure that calculates the state derivative, the initial state, the increment of the independent variable, and the relative error tolerance allowed in the new state.[62]

```
(define plot-win (frame 0. 100. -pi pi))

(define (do-it sysder initial-istate final-time dt tolerance)
  (let loop ((istate initial-istate))
    (if (< (istate->t istate) final-time)
      (let ((ns (ode-advancer sysder istate dt tolerance)))
        (let ((local (istate->local ns)))
          (let ((theta
                  ((principal-value pi) (coordinate local))))
            (plot-point plot-win (time local) theta)))
        (loop ns)))))

(do-it (pend-sysder-compiled
         1.0                          ;m=1kg
         1.0                          ;l=1m
         9.8                          ;g=9.8m/s^2
         0.1                          ;a=1/10 m
         (* 2.0 (sqrt 9.8)) )         ;omega=2*omega_0
       (->istate 0.0                  ;t_0=0
                 1.0                  ;theta_0=1 radian
                 0.0)                 ;thetadot_0=0 radians/s
       100.0                          ;final time
       0.01                           ;step between plotted points
       1.0e-15)                       ;max local truncation error
```

Figure (1.7) shows the angle θ versus time for a couple of orbits for the driven pendulum. The initial conditions for the two runs are the same except that in one the bob is given a tiny velocity equal to 10^{-10}m/s, about one atom width per second. The initial segments of the two orbits are indistinguishable. After about 75 seconds the two orbits diverge and become completely different.

[62]The results are plotted in a plot-window which is created by the procedure `frame` with arguments `xmin`, `xmax`, `ymin`, `ymin`, that specify the limits of the plotting area. Points are added to the plot with the procedure `plot-point` that takes a plot-window and the abscissa and ordinate of the point to be plotted.

The procedure `principal-value` is used to reduce an angle to a standard interval. The argument to `principal-value` is the point at which the circle is to be cut. Thus `(principal-value pi)` is a procedure that reduces an angle θ to the interval $-\pi \leq \theta < \pi$.

The procedure `istate->t` extracts the time component from an integrator state.

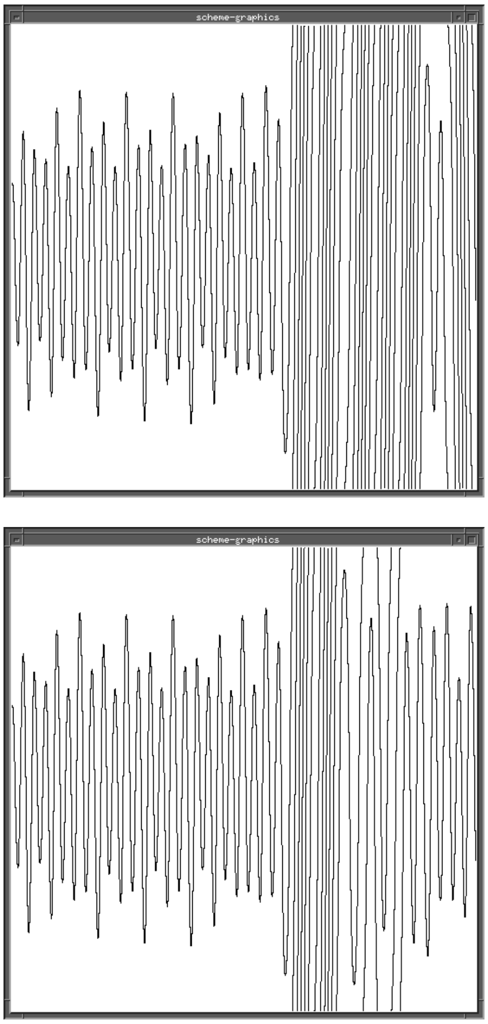

Figure 1.7 Orbits of the driven pendulum. The angle θ is plotted on the vertical axis in the interval $(-\pi, \pi)$. Time is plotted on the horizontal axis. Because angles are periodic, this plot may be thought of as wound around a cylinder. (Top) This simulation uses initial conditions $\theta = 1$ and $\dot{\theta} = 0$. The orbit oscillates for a while, then circulates, then begins to circulate in the opposite direction. (Bottom) Here we use a slightly different initial angular velocity, $\dot{\theta} = 10^{-10}$. The initial behavior is indistinguishable from the top figure, but the two trajectories become uncorrelated after the transition between oscillation and circulation. This extreme sensitivity to initial conditions is characteristic of systems with chaotic behavior.

This extreme sensitivity to tiny changes in initial conditions is characteristic of what is called *chaotic behavior*. Later, we will investigate this example further, using other tools such as Lyapunov exponents, phase space, and Poincaré sections.

1.9 Conserved Quantities

A quantity which is a function of the local state of the system that is constant along a solution path is called a *conserved quantity* or a *constant of motion*. If C is a conserved quantity, then

$$D(C \circ \Gamma[q]) = D_t C \circ \Gamma[q] = 0 \tag{1.111}$$

for solution paths q. Following historical practice we also refer to constants of the motion as *integrals* of the motion.[63] In this section, we will investigate systems with symmetry and find that symmetries are associated with conserved quantities. For instance, linear momentum is conserved in a system with translational symmetry, angular momentum is conserved if there is rotational symmetry, energy is conserved if the system does not depend on the origin of time. We first consider systems for which a coordinate system can be chosen that naturally expresses the symmetry, and later discuss systems for which no coordinate system can be chosen that simultaneously expresses all symmetries.

1.9.1 Conserved momenta

If a Lagrangian $L(t, q, v)$ does not depend on some particular coordinate q^i, then

$$(\partial_1 L)_i = 0, \tag{1.112}$$

and the corresponding ith component of the Lagrange equations is

$$(D(\partial_2 L \circ \Gamma[q]))_i = 0. \tag{1.113}$$

[63] In the older literature conserved quantities are sometimes called *first integrals*.

This is the same as[64]

$$D\left((\partial_2 L)_i \circ \Gamma[q]\right) = 0. \tag{1.114}$$

So we see that

$$\mathcal{P}_i = (\partial_2 L)_i \tag{1.115}$$

is a conserved quantity. The function $\mathcal{P}_i$ is called the *momentum state function*. Its value is constant along realizable paths; it may have different values on different paths. The value of the momentum state function is the *generalized momentum*. We refer to ith component of the generalized momentum as the momentum *conjugate* to the ith coordinate.[65] A generalized coordinate component that does not appear explicitly in the Lagrangian is called a *cyclic coordinate*. The generalized momentum component conjugate to any cyclic coordinate is a constant of the motion. As we will see, momentum is an important quantity even when it is not conserved.

Given the coordinate path q and the Lagrangian L, the momentum path p is

$$p = \partial_2 L \circ \Gamma[q] = \mathcal{P} \circ \Gamma[q], \tag{1.116}$$

with components

$$p_i = \mathcal{P}_i \circ \Gamma[q]. \tag{1.117}$$

The momentum path is well defined for any path q. If the path is realizable and the Lagrangian does not depend on q^i then p_i is a constant function

$$Dp_i = 0. \tag{1.118}$$

The constant value of p_i may be different for different trajectories.

[64] The derivative of a component is equal to the component of the derivative.

[65] Observe that we indicate a component of the generalized momentum with a subscript, and indicate a component of the generalized coordinates with a superscript. These conventions are consistent with the ones that are commonly used in tensor algebra, which is sometimes helpful in working out complex problems.

Examples of Conserved Momenta

The free particle Lagrangian $L(t, x, v) = \frac{1}{2}mv^2$ is independent of x. So the momentum state function, $\mathcal{P}(t, q, v) = mv$, is conserved along realizable paths. The momentum path p for the coordinate path q is $p(t) = \mathcal{P} \circ \Gamma[q](t) = m\, Dq(t)$. For a realizable path $Dp(t) = 0$. For the free particle the usual linear momentum is conserved for realizable paths.

For a particle in a central force field (section 1.6), the Lagrangian

$$L(t; r, \varphi; \dot{r}, \dot{\varphi}) = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\varphi}^2) - V(r)$$

depends on r but is independent of φ. The momentum state-function is

$$\mathcal{P}(t; r, \varphi; \dot{r}, \dot{\varphi}) = \left[m\dot{r}, mr^2\dot{\varphi}\right].$$

It has two components. The first component, "the radial momentum," is not conserved. The second component, "the angular momentum," is conserved along any solution trajectory.

If the central potential problem had been expressed in rectangular coordinates, then all of the coordinates would have appeared in the Lagrangian. In that case there would not be any obvious conserved quantities. Nevertheless, the motion of the system does not depend on the choice of coordinates; so the angular momentum is still conserved.

We see that there is great advantage in making a judicious choice for the coordinate system. If we can choose the coordinates so that a symmetry of the system is reflected in the Lagrangian by the absence of some coordinate component, then the existence of a corresponding conserved quantity will be automatic.[66]

1.9.2 Energy and energy conservation

Momenta are conserved by the motion if the Lagrangian does not depend on the corresponding coordinate. There is another con-

[66] In general, conserved quantities in a physical system are associated with continuous symmetries, whether or not one can find a coordinate system in which the symmetry is apparent. This powerful notion was formalized and a theorem linking conservation laws with symmetries was proved by E. Noether early in the 20th century. See section 1.9.4 on Noether's theorem.

stant of the motion, the energy, if the Lagrangian $L(t, q, \dot{q})$ does not depend explicitly on the time: $\partial_0 L = 0$.

Consider the time derivative of the Lagrangian along a solution path q:

$$D(L \circ \Gamma[q]) = \partial_0 L \circ \Gamma[q] + (\partial_1 L \circ \Gamma[q]) Dq + (\partial_2 L \circ \Gamma[q]) D^2 q. \quad (1.119)$$

Using Lagrange's equations to rewrite the second term

$$D(L \circ \Gamma[q]) = (\partial_0 L) \circ \Gamma[q] + D(\partial_2 L \circ \Gamma[q]) Dq + (\partial_2 L \circ \Gamma[q]) D^2 q. \quad (1.120)$$

Isolating $\partial_0 L$ and combining the first two terms on the right side

$$\begin{aligned}(\partial_0 L) \circ \Gamma[q] &= D(L \circ \Gamma[q]) - D((\partial_2 L \circ \Gamma[q]) Dq) \\ &= D(L \circ \Gamma[q]) - D((\partial_2 L \circ \Gamma[q])(\dot{Q} \circ \Gamma[q])) \\ &= D((L - \mathcal{P}\dot{Q}) \circ \Gamma[q]),\end{aligned} \quad (1.121)$$

where, as before, $\dot{Q}$ selects the velocity from the state. So we see that if $\partial_0 L = 0$ then

$$\mathcal{E} = \mathcal{P}\dot{Q} - L, \quad (1.122)$$

is a conserved along realizable paths. The function $\mathcal{E}$ is called the *energy state function*.[67] Let $E = \mathcal{E} \circ \Gamma[q]$ denote the energy function on the path q. The energy function has a constant value along any realizable trajectory if the Lagrangian has no explicit time dependence; the energy E may have a different value for different trajectories. A system that has no explicit time dependence is called *autonomous*.

Given a Lagrangian `L`, we may compute the energy:

```
(define (Lagrangian->energy L)
  (let ((P ((partial 2) L)))
    (- (* P velocity) L)))
```

Energy in terms of Kinetic and Potential Energies

In some cases the energy can be written as the sum of kinetic and potential energies. Suppose the system is composed of particles with rectangular coordinates $\mathbf{x}_\alpha$, the movement of which may be subject to constraints, and that these rectangular coordinates are some functions of the generalized coordinates q and possibly time

[67] The sign of the energy state function is a matter of convention.

t: $\mathbf{x}_\alpha = f_\alpha(t, q)$. We form the Lagrangian as $L = T - V$ and compute the kinetic energy in terms of q by writing the rectangular velocities in terms of the generalized velocities:

$$\mathbf{v}_\alpha = \partial_0 f_\alpha(t, q) + \partial_1 f_\alpha(t, q) v. \tag{1.123}$$

The kinetic energy is

$$T(t, q, v) = \tfrac{1}{2} \textstyle\sum_\alpha m_\alpha v_\alpha^2, \tag{1.124}$$

where v_α is the magnitude of $\mathbf{v}_\alpha$.

If the f_α functions do not depend explicitly on time ($\partial_0 f_\alpha = 0$), then the rectangular velocities are homogeneous functions of the generalized velocities of degree 1, and T is a homogeneous function of the generalized velocities of degree 2, because it is formed by summing the square of homogeneous functions of degree 1. For the special case when T is a homogeneous function of degree 2 in the generalized velocities, then

$$\mathcal{P}\dot{Q} = (\partial_2 T)\dot{Q} = 2T, \tag{1.125}$$

where the second equality follows from Euler's theorem on homogeneous functions.[68] The energy state function is

$$\mathcal{E} = \mathcal{P}\dot{Q} - L = \mathcal{P}\dot{Q} - T + V. \tag{1.126}$$

So if f_α is independent of time, the energy function can be rewritten

$$\mathcal{E} = 2T - T + V = T + V. \tag{1.127}$$

Notice that if V depends on time the energy is still the sum of the kinetic energy and potential energy, but the energy is not conserved.

The energy state function is always a well defined function, whether or not it can be written in the form of $T + V$, and whether or not it is conserved along realizable paths.

---

[68] Euler's theorem says that if f is a function of $x = (x_0, x_1, \ldots)$ that is homogeneous of degree n in each of the x_i, then

$$\sum_i \left(\frac{\partial f}{\partial x_i}(x) x_i \right) = n f(x).$$

Exercise 1.30:
An analogous result holds when the f_α do depend explicitly on time.

a. Show that in this case the kinetic energy contains terms that are linear in the generalized velocities.

b. Show that, by adding a total time derivative, the Lagrangian can be written in the form $L = A - B$, where A is a homogeneous quadratic form in the generalized velocities, and B is velocity independent.

c. Show, using Euler's theorem, that the energy function is $\mathcal{E} = A + B$.
An example where terms that were linear in the velocity were removed from the Lagrangian by adding a total time derivative has already been given: the driven pendulum.

1.9.3 Central forces in 3 dimensions

One important physical system is the motion of a particle in a central field in three dimensions, with an arbitrary potential energy $V(r)$ depending only on the radius. We will describe this system in spherical coordinates r, θ, and φ, where θ is the colatitude and φ is the longitude. The kinetic energy has three terms:

$$T(t; r, \theta, \varphi; \dot{r}, \dot{\theta}, \dot{\varphi}) = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2 + r^2(\sin\theta)^2\dot{\varphi}^2).$$

As a procedure:

```
(define ((T3-spherical m) local)
  (let ((t (time local))
        (q (coordinate local))
        (qdot (velocity local)))
    (let ((r (ref q 0))
          (theta (ref q 1))
          (phi (ref q 2))
          (rdot (ref qdot 0))
          (thetadot (ref qdot 1))
          (phidot (ref qdot 2)))
      (* 1/2 m
        (+ (square rdot)
           (square (* r thetadot))
           (square (* r (sin theta) phidot)))))))
```

The Lagrangian is then formed by subtracting the potential energy:

```
(define (L3-central m Vr)
  (define (Vs local)
    (let ((r (ref (coordinate local) 0)))
      (Vr r)))
  (- (T3-spherical m) Vs))
```

Let's first look at the generalized forces (the derivatives of the Lagrangian with respect to the generalized coordinates). We compute these with a partial derivative with respect to the coordinate argument of the Lagrangian:

```
(show-expression
 (((partial 1) (L3-central 'm (literal-function 'V)))
  (->local 't
           (coordinate-tuple 'r 'theta 'phi)
           (velocity-tuple 'rdot 'thetadot 'phidot))))
```

$$\begin{bmatrix} m\dot{\varphi}^2 r\,(\sin(\theta))^2 + mr\dot{\theta}^2 - DV(r) \\ m\dot{\varphi}^2 r^2 \cos(\theta)\sin(\theta) \\ 0 \end{bmatrix}$$

The φ component of the force is zero because φ does not appear in the Lagrangian (it is a cyclic variable). The corresponding momentum component is conserved. Compute the momenta:

```
(show-expression
 (((partial 2) (L3-central 'm (literal-function 'V)))
  (->local 't
           (coordinate-tuple 'r 'theta 'phi)
           (velocity-tuple 'rdot 'thetadot 'phidot))))
```

$$\begin{bmatrix} m\dot{r} \\ mr^2\dot{\theta} \\ mr^2\dot{\varphi}\,(\sin(\theta))^2 \end{bmatrix}$$

The momentum conjugate to φ is conserved. This is the z component of the angular momentum $\vec{r} \times (m\vec{v})$, for vector position $\vec{r}$ and linear momentum $m\vec{v}$. We can show this by writing the z component of the angular momentum in spherical coordinates:

```
(define ((ang-mom-z m) local)
  (let ((q (coordinate local))
        (v (velocity local)))
     (ref (cross-product q (* m v)) 2)))

(define (s->r t q)
  (let ((r (ref q 0))
        (theta (ref q 1))
        (phi (ref q 2)))
    (let ((x (* r (sin theta) (cos phi)))
          (y (* r (sin theta) (sin phi)))
          (z (* r (cos theta))))
      (coordinate-tuple x y z))))

(show-expression
  ((compose (ang-mom-z 'm) (F->C s->r))
   (->local 't
            (coordinate-tuple 'r 'theta 'phi)
            (velocity-tuple 'rdot 'thetadot 'phidot))))
```

$$m r^2 \dot{\varphi} \left(\sin\left(\theta\right)\right)^2$$

The choice of the z-axis is arbitrary, so the conservation of any component of the angular momentum implies the conservation of all components. Thus the total angular momentum is conserved. We can choose the z axis so all of the angular momentum is in the z component. The angular momentum must be perpendicular to both the radius vector and to the linear momentum vector. Thus the motion is planar, $\theta = \pi/2$, and $\dot{\theta} = 0$. Planar motion in a central-force field was discussed in section 1.6.

We can also see that the energy state function computed from the Lagrangian for a central field is in fact $T + V$:

```
(show-expression
 ((Lagrangian->energy (L3-central 'm (literal-function 'V)))
  (->local 't
           (coordinate-tuple 'r 'theta 'phi)
           (velocity-tuple 'rdot 'thetadot 'phidot))))
```

$$\frac{1}{2} m \dot{\varphi}^2 r^2 \left(\sin\left(\theta\right)\right)^2 + \frac{1}{2} m r^2 \dot{\theta}^2 + \frac{1}{2} m \dot{r}^2 + V\left(r\right)$$

The energy is conserved because the Lagrangian has no explicit time dependence.

Exercise 1.31: Driven Spherical Pendulum

A spherical pendulum is a massive bob, subject to uniform gravity, that may swing in three dimensions, but remains at a given distance from the pivot. Formulate a Lagrangian for a spherical pendulum, driven by vertical motion of the pivot. What symmetry(ies) can you find? Find coordinates that express the symmetry. What is conserved? Give analytic expression(s) for the conserved quantity(ies).

1.9.4 Noether's Theorem

We have seen that if a system has a symmetry and if a coordinate system can be chosen so that the Lagrangian does not depend on the coordinate associated with the symmetry then there is a conserved quantity associated with the symmetry. In this section we show that continuous symmetries correspond to conserved quantities with any choice of coordinate system.

What does it mean to say that a system has a continuous symmetry? Informally, a system has a symmetry if the equations of motion are unchanged by a coordinate transformation corresponding to the symmetry. A continuous symmetry is a parametric family of symmetries. Consider a parametric coordinate transformation $\widetilde{T}$ with parameter s:

$$q = \widetilde{T}(s)(t, q'). \tag{1.128}$$

We assume the transformations $\widetilde{T}(s)$ have no dependence on the generalized velocities.[69] To this parametric coordinate transformation there corresponds a parametric state transformation $\widetilde{C}$:

$$(t, q, v) = \widetilde{C}(s)(t, q', v'). \tag{1.129}$$

We require that the transformation $\widetilde{T}(0)$ is the identity coordinate transformation $q' = \widetilde{T}(0)(t, q')$; and as a consequence $\widetilde{C}(0)$ is the identity state transformation $(t, q', v') = \widetilde{C}(0)(t, q', v')$. We say that a Lagrangian has a continuous symmetry corresponding to $\widetilde{T}$ if

$$\widetilde{L}(s) = L \circ \widetilde{C}(s) = L \tag{1.130}$$

[69] Noether's theorem is more general than we state and prove it here. Properly, we should also consider velocity dependent symmetries.

for any s. That is, $\widetilde{T}$ is a continuous symmetry of L if the Lagrangian L is the same function as the transformed Lagrangian $\widetilde{L}(s)$. Explicitly,

$$\widetilde{L}(s)(t,q',v') = L(t,\widetilde{T}(s)(t,q'),D_t(\widetilde{T}(s))(t,q',v')), \tag{1.131}$$

where we have rewritten the velocity component of $\widetilde{C}(s)$ in terms of the total time derivative.

That $\widetilde{L}(s) = L$ for any s implies $D\widetilde{L}(s) = 0$:

$$\begin{aligned}0 &= D\widetilde{L}(s)(t,q',v')\\ &= \partial_1(\widetilde{L}(s))(t,q',v')(D\widetilde{T})(s)(t,q')\\ &\quad + \partial_2(\widetilde{L}(s))(t,q',v')D_t(D\widetilde{T}(s))(t,q').\end{aligned} \tag{1.132}$$

On a solution path q', we can use the Lagrange equations to rewrite the first term

$$\begin{aligned}0 &= D(\partial_2(\widetilde{L}(s))\circ\Gamma[q'])(D\widetilde{T})(s)\circ\Gamma[q']\\ &\quad + \partial_2(\widetilde{L}(s))\circ\Gamma[q']D_t(D\widetilde{T}(s))\circ\Gamma[q']\\ &= ((D_t(\partial_2(\widetilde{L}(s))))((D\widetilde{T})(s)) + (\partial_2(\widetilde{L}(s)))D_t(D\widetilde{T}(s)))\circ\Gamma[q']\\ &= D_t((\partial_2(\widetilde{L}(s)))(D\widetilde{T}(s)))\circ\Gamma[q'].\end{aligned} \tag{1.133}$$

Thus

$$I(s) = (\partial_2(\widetilde{L}(s)))(D\widetilde{T}(s)), \tag{1.134}$$

is conserved along solution trajectories. In particular, for $s = 0$,

$$\mathcal{I} = I(0) = (\partial_2 L)(D\widetilde{T}(0)) \tag{1.135}$$

is a conserved quantity. This is Noether's integral. The integral is the product of the momentum and a vector associated with the symmetry.

Illustration: Motion in a Central Potential

For example, consider the central potential Lagrangian in rectangular coordinates:

$$\begin{aligned}&L(t;x,y,z;v_x.v_y,v_z)\\ &\qquad = \tfrac{1}{2}m\left(v_x^2+v_y^2+v_z^2\right) - V\left(\sqrt{x^2+y^2+z^2}\right),\end{aligned} \tag{1.136}$$

and a parametric rotation $\widetilde{R}_z(s)$ about the z axis

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \widetilde{R}_z(s) \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} \cos s & \sin s & 0 \\ -\sin s & \cos s & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix}. \tag{1.137}$$

The rotation is an orthogonal transformation so

$$x^2 + y^2 + z^2 = (x')^2 + (y')^2 + (z')^2. \tag{1.138}$$

Differentiating along a path, we get

$$\begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} = \widetilde{R}_z(s) \begin{bmatrix} v'_x \\ v'_y \\ v'_z \end{bmatrix}, \tag{1.139}$$

so the velocities also transform by an orthogonal transformation, and $v_x^2 + v_y^2 + v_z^2 = (v'_x)^2 + (v'_y)^2 + (v'_z)^2$. Thus

$$\begin{aligned} &L'(t; x', y', z'; v'_x, v'_y, v'_z) \\ &\quad = \tfrac{1}{2} m \left((v'_x)^2 + (v'_y)^2 + (v'_z)^2 \right) \\ &\qquad - V\left(\sqrt{(x')^2 + (y')^2 + (z')^2} \right), \end{aligned} \tag{1.140}$$

and we see that L' is precisely the same function as L.

The momenta are

$$\partial_2 L(t; x, y, z; v_x, v_y, v_z) = [m v_x, m v_y, m v_z]. \tag{1.141}$$

and

$$\begin{aligned} D\widetilde{T}(0)(t; x, y, z) &= D\widetilde{R}_z(0) \begin{bmatrix} x \\ y \\ z \end{bmatrix} \\ &= \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}. \end{aligned} \tag{1.142}$$

So the Noether integral is

$$\begin{aligned} \mathcal{I}(t; x, y, z; v_x, v_y, v_z) &= ((\partial_2 L)(D\widetilde{T}(0)))(t; x, y, z; v_x, v_y, v_z) \\ &= m(y v_x - x v_y), \end{aligned} \tag{1.143}$$

which we recognize as minus the z component of the angular momentum: $\vec{x} \times (m\vec{v})$. Since the Lagrangian is preserved by any continuous rotational symmetry, all components of the vector angular momenta are conserved for the central potential problem.

1.10 Constrained Motion

An advantage of the Lagrangian approach is that the coordinates can often be chosen to exactly describe the freedom of the system, automatically incorporating any constraints. We may also use coordinates that have more freedom than the system actually has and consider explicit constraints among the coordinates. For example, the planar pendulum has a one-dimensional configuration space. We have formulated this problem using the angle from the vertical as the configuration coordinate. Alternatively, we may choose to represent the pendulum as a moving body in the plane, constrained to be on the circle of the correct radius around the pivot. We would like to have valid descriptions for both choices and show they are equivalent. In this section we develop tools to handle problems with explicit constraints. The constraints considered here are more general than those considered in the demonstration that the Lagrangian for systems with rigid constraints can be written as the difference of kinetic and potential energies (see Section 1.6.2).

Suppose that the configuration of a system with n degrees of freedom is specified by $n+1$ coordinates that are constrained to satisfy some relation

$$\varphi(t, q, v) = 0. \tag{1.144}$$

How do we formulate the equations of motion? One approach would be to use the constraint equation to eliminate one of the coordinates in favor of the rest, and then the evolution of the reduced set of generalized coordinates would be described by the usual Lagrange equations. The equations governing the evolution of coordinates that are not fully independent should be equivalent.

We can address the problem of formulating equations of motion for systems with redundant coordinates by returning to the action principle. Realizable paths are distinguished from other paths by having stationary action. Stationary refers to the fact that the action does not change with certain small variations of the path. What variations should be considered? We have seen that velocity-independent rigid constraints can be used to eliminate redundant coordinates. In the non-redundant coordinates we distinguished realizable paths using variations that by construction satisfy the constraints. Thus in the case where constraints can be used to eliminate redundant coordinates we can restrict the variations in the path to those that are consistent with the constraints.

So how does the restriction of the possible variations affect the argument that led to Lagrange's equations (refer to section 1.5)? Actually most of the calculation is unaffected. The condition that the action is stationary still reduces to the condition (1.33):

$$0 = \int_{t_1}^{t_2} \left\{ (\partial_1 L \circ \Gamma[q]) - D(\partial_2 L \circ \Gamma[q]) \right\} \eta. \tag{1.145}$$

At this point we argued that because the variations η are arbitrary (except for conditions at the endpoints), the only way for the integral to be zero is for the integrand to be zero. Furthermore, the freedom in our choice of η allowed us to deduce that the factor multiplying η in the integrand must be identically zero, thereby deriving Lagrange's equations.

Now the choice of η is not completely free. We may still deduce from the arbitrariness of η that the integrand must be zero,[70] but we may no longer deduce that the factor multiplying η is zero (only that the projection of this factor onto acceptable variations is zero). So we have

$$\left\{ (\partial_1 L \circ \Gamma[q]) - D(\partial_2 L \circ \Gamma[q]) \right\} \eta = 0, \tag{1.146}$$

with η subject to the constraints.

A path q satisfies the constraint $\varphi = 0$ if $\bar{\varphi}[q] = \varphi \circ \Gamma[q] = 0$. The constraint must be satisfied even for the varied path, so we only allow variations η for which the variation of the constraint is zero:

$$\delta_\eta(\bar{\varphi}) = 0. \tag{1.147}$$

[70] Given any acceptable variation we may make another acceptable variation by multiplying the given one by a bump function that emphasizes any particular time interval.

We can say that the variation must be "tangent" to the constraint surface. Expanding this with the chain rule, a variation η is tangent to the constraint surface φ if

$$(\partial_1 \varphi \circ \Gamma[q]) \ \eta + (\partial_2 \varphi \circ \Gamma[q]) \ D\eta = 0. \tag{1.148}$$

Note that these are functions of time; the variation at a given time is tangent to the constraint at that time.

1.10.1 Coordinate Constraints

Consider constraints that do not depend on velocities:

$$\partial_2 \varphi \equiv 0.$$

In this case the variation is tangent to the constraint surface if

$$(\partial_1 \varphi \circ \Gamma) \ \eta = 0. \tag{1.149}$$

Together, equations (1.146) and (1.149) should determine the motion, but how do we eliminate η? The residual of the Lagrange equations is orthogonal[71] to any η that is orthogonal to the normal to the constraint surface. A vector that is orthogonal to all vectors orthogonal to a given vector is parallel to the given vector. Thus, the residual of Lagrange's equations is parallel to the normal to the constraint surface; the two must be proportional:

$$D\left(\partial_2 L \circ \Gamma[q]\right) - \partial_1 L \circ \Gamma[q] = \lambda(\partial_1 \varphi) \circ \Gamma[q]. \tag{1.150}$$

That the two vectors are parallel everywhere along the path does not guarantee that the proportionality factor is the same at each moment along the path, so the proportionality factor λ is some function of time, which may depend on the path under consideration. These equations, with the constraint equation $\varphi \circ \Gamma[q] = 0$, are the governing equations. These equations are sufficient to determine the path q and to eliminate the unknown function λ.

[71] We take two tuple-valued functions of time to be orthogonal if at each instant the dot product of the tuples is zero. Similarly, tuple-valued functions are considered parallel if at each moment one of the tuples is a scalar multiple of the other. The scalar multiplier is in general a function of time.

Now watch this

Suppose we form an augmented Lagrangian treating λ as one of the coordinates

$$L'(t; q, \lambda; \dot{q}, \dot{\lambda}) = L(t, q, \dot{q}) + \lambda\varphi(t, q, \dot{q}). \tag{1.151}$$

The Lagrange equations associated with the coordinates q are just the modified Lagrange equations (1.150), and the Lagrange equation associated with λ is just the constraint equation. (Note that $\dot{\lambda}$ does not appear in the augmented Lagrangian.) So the Lagrange equations for this augmented Lagrangian fully encapsulate the modification to the Lagrange equations that is imposed by the addition of an explicit coordinate constraint, at the expense of introducing extra degrees of freedom. Notice that this Lagrangian is of the same form as Lagrangian (1.69) that we used in the derivation of $L = T - V$ for rigid systems (Section 1.6.2).

Alternatively

How do we know that we have enough information to eliminate the unknown function λ from equations (1.150) or that the extra degree of freedom introduced in Lagrangian (1.151) is purely formal?

If λ could be written as a function of the solution state path, then it would be clear that it is determined by the state and can thus be eliminated. Okay, suppose λ can be written as a composition of state-dependent function with the path: $\lambda = \Lambda \circ \Gamma[q]$. Consider the Lagrangian

$$L'' = L + \Lambda\varphi. \tag{1.152}$$

This new Lagrangian has no extra degrees of freedom. The Lagrange equations for L'' are the Lagrange equations for L with additional terms arising from the product of $\Lambda\varphi$. Applying the Euler-Lagrange operator E (see section 1.7) to this Lagrangian gives[72]

$$\begin{aligned} \mathsf{E}\left[L''\right] &= \mathsf{E}\left[L\right] + \mathsf{E}\left[\Lambda\varphi\right] \\ &= \mathsf{E}\left[L\right] + \Lambda\,\mathsf{E}\left[\varphi\right] + \mathsf{E}\left[\Lambda\right]\,\varphi + D_t\Lambda\,\partial_2\varphi + \partial_2\Lambda\,D_t\varphi. \end{aligned} \tag{1.153}$$

[72]Recall that the Euler-Lagrange operator E has the property

$$\mathsf{E}\left[FG\right] = F\,\mathsf{E}[G] + \mathsf{E}[F]\,G + D_tF\,\partial_2 G + \partial_2 F\,D_t G.$$

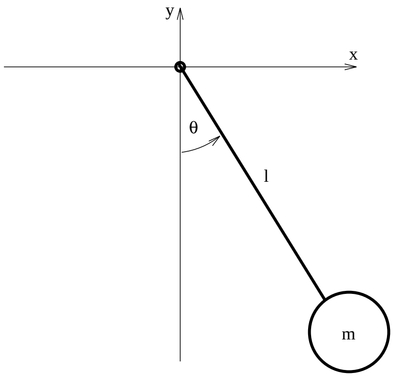

Figure 1.8 We can formulate the behavior of a pendulum as motion in the plane, constrained to a circle about the pivot.

Composition of $\mathsf{E}[L'']$ with $\Gamma[q]$ gives the Lagrange equations for the path q. Using the fact that the constraint is satisfied on the path $\varphi \circ \Gamma[q] = 0$ and consequently $D_t\varphi \circ \Gamma[q] = 0$, we have

$$\mathsf{E}\left[L''\right] \circ \Gamma[q] = (\mathsf{E}\left[L\right] + \lambda \mathsf{E}\left[\varphi\right] + D\lambda(\partial_2\varphi)) \circ \Gamma[q], \tag{1.154}$$

where we have used $\lambda = \Lambda \circ \Gamma[q]$. If we now use the fact that we are only dealing with coordinate constraints, $\partial_2\varphi = 0$ then

$$\mathsf{E}\left[L''\right] \circ \Gamma[q] = (\mathsf{E}\left[L\right] + \lambda \mathsf{E}[\varphi]) \circ \Gamma[q]. \tag{1.155}$$

The Lagrange equations are the same as those derived from the augmented Lagrangian L'. The difference is that now we see that $\lambda = \Lambda \circ \Gamma[q]$ is determined by the unaugmented state. This is the same as saying that λ can be eliminated.

Considering only the formal validity of the Lagrange equations for the augmented Lagrangian, we could not deduce that λ could be written as the composition of a state-dependent function Λ with $\Gamma[q]$. The explicit Lagrange equations derived from the augmented Lagrangian depend on the accelerations D^2q as well as λ so we may not deduce separately that either is the composition of a state-dependent function and $\Gamma[q]$. However, now we see that λ is such a composition. This allows us to deduce that D^2q is also a state-dependent function composed with the path. The evolution of the system is determined from the dynamical state.

The pendulum using constraints

The pendulum can be formulated as the motion of a massive particle in a vertical plane subject to the constraint that the distance to the pivot is constant (see figure 1.8).

In this formulation, the kinetic and potential energies in the Lagrangian are those of an unconstrained particle in a uniform gravitational acceleration. A Lagrangian for the unconstrained particle is

$$L(t; x, y; v_x, v_y) = \frac{1}{2}m(v_x^2 + v_y^2) - mgy. \tag{1.156}$$

The constraint that the pendulum moves in a circle of radius l about the pivot is[73]

$$x^2 + y^2 - l^2 = 0. \tag{1.157}$$

The augmented Lagrangian is

$$L'(t; x, y, \lambda; v_x, v_y, \dot{\lambda}) = \frac{1}{2}m(v_x^2+v_y^2) - mgy + \lambda(x^2+y^2-l^2). \tag{1.158}$$

The Lagrange equations for the augmented Lagrangian are

$$mD^2x - 2\lambda x = 0 \tag{1.159}$$
$$mD^2y + mg - 2\lambda y = 0. \tag{1.160}$$
$$x^2 + y^2 - l^2 = 0 \tag{1.161}$$

These equations are sufficient to solve for the motion of the pendulum.

It should not be surprising that these equations simplify if we switch to "polar" coordinates

$$x = r\sin\theta \qquad y = -r\cos\theta. \tag{1.162}$$

Substituting this into the constraint equation we determine that $r = l$, a constant. Forming the derivatives and substituting into the other two equations we find

$$ml(\cos\theta D^2\theta - \sin\theta(D\theta)^2) - 2\lambda\sin\theta = 0 \tag{1.163}$$
$$ml(\sin\theta D^2\theta + \cos\theta(D\theta)^2) + mg + 2\lambda\cos\theta = 0. \tag{1.164}$$

[73] This constraint has the same form as the constraints used in the demonstration that $L = T - V$ can be used for rigid systems. Here it is a particular example of a more general set of constraints.

Multiplying the first by $\cos\theta$ and the second by $\sin\theta$ and adding, we find

$$mlD^2\theta + mg\sin\theta = 0, \tag{1.165}$$

which we recognize as the correct equation for the pendulum. This is the same as the Lagrange equation for the pendulum using the unconstrained generalized coordinate θ. For completeness, we can find λ in terms of the other variables

$$\lambda = \frac{mD^2x}{2x} = -\frac{1}{2l}(mg\cos\theta + ml(D\theta)^2). \tag{1.166}$$

This confirms that λ is really the composition of a function of the state with the state path. Notice that $2l\lambda$ is a force – it is the sum of the outward component of the gravitational force and the centrifugal force. Using this interpretation in the two coordinate equations of motion we see that the terms involving λ are the forces that must be applied to the unconstrained particle to make it move on the circle required by the constraints. Equivalently, we may think of $2l\lambda$ as the tension in the pendulum rod that holds the mass.[74]

Building systems from parts

The method of using augmented Lagrangians to enforce constraints on dynamical systems provides us with a way of building the analysis of a compound system by combining the results of the analysis of the parts of the system and the coupling between them. Consider the compound spring-mass system shown in figure 1.9. We could analyze this as a monolithic system with two configuration coordinates x_1 and x_2. An alternative is to analyze the basic unit with an extra configuration coordinate x_c and then impose a constraint $x_c = x_1$ to accomplish the coupling.

Let X_i be the equilibrium position of the ith spring. The Lagrangian for the subsystem attached to the wall is

$$L_1(t, x_1, \dot{x}_1) = \tfrac{1}{2}m_1\dot{x}_1^2 - \tfrac{1}{2}k_1(x_1 - X_1)^2 \tag{1.167}$$

[74]Indeed, if we had scaled the constraint equations as we did in the discussion of Newtonian constraint forces we could have identified λ with the the magnitude of the constraint force F. However, though λ will in general be related to the constraint forces it will not be one of them. We chose to leave the scaling as it naturally appeared rather than make things turn out artificially pretty.

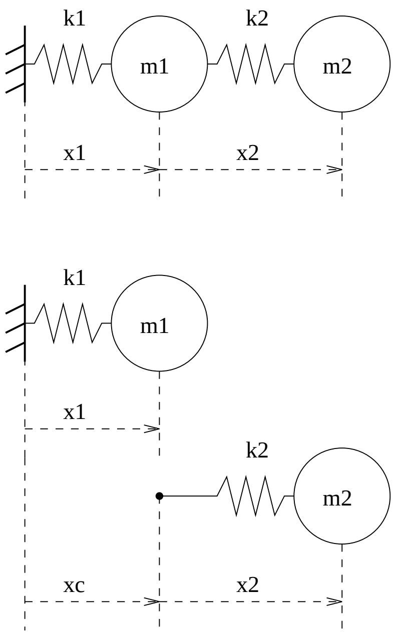

Figure 1.9 A compound spring-mass system is decomposed into two subsystems. We have two springs and masses that may only move horizontally. The equilibrium positions of the springs are X_1 and X_2. The systems are coupled by the position-coordinate constraint $x_c = x_1$.

and the Lagrangian for the subsystem that attaches to it is

$$L_2(t; x_c, x_2; \dot{x}_c, \dot{x}_2) = \tfrac{1}{2} m_2 (\dot{x}_c + \dot{x}_2)^2 - \tfrac{1}{2} k_2 (x_2 - X_2)^2. \tag{1.168}$$

This could be a repeated subunit in a much more complex system.

The Lagrangian for the system composed from these parts is a sum of each of the separate parts and the coupling term:

$$\begin{aligned} L(t; x_1, x_2, x_c, \lambda; \dot{x}_1, \dot{x}_2, \dot{x}_c, \dot{\lambda}) = {} & L_1(t, x_1, \dot{x}_1) \\ & + L_2(t; x_c, x_2; \dot{x}_c, \dot{x}_2) \\ & + \lambda(x_c - x_1) \end{aligned} \tag{1.169}$$

Thus we can write Lagrange's equations as follows:

$$m_1 D^2 x_1 = -k_1(x_1 - X_1) + \lambda \tag{1.170}$$

$$m_2(D^2 x_c + D^2 x_2) = -k_2(x_2 - X_2) \tag{1.171}$$

$$m_2(D^2 x_c + D^2 x_2) = -\lambda \tag{1.172}$$

These three equations, combined with the original constraint

$$x_c = x_1, \tag{1.173}$$

(which is the Lagrange equation for the coordinate λ), are sufficient to solve for the three configuration coordinates and λ. Notice that in this system λ is the force of constraint, holding the system together.

Exercise 1.32: Bead on a Triaxial Surface

Consider again the motion of a bead constrained to move on a triaxial surface from Exercise 1.20. Reformulate this using rectangular coordinates as the generalized coordinates with an explicit constraint that the bead stay on the surface. Find a Lagrangian and show that the Lagrange equations are equivalent to those found in Exercise 1.20.

Exercise 1.33: Motion of a Tiny Golf Ball

Consider the motion of a golf ball idealized as a point mass constrained to a frictionless smooth surface of varying height $h(x, y)$ in a uniform gravitational field with acceleration g.

a. Find an augmented Lagrangian for this system, and derive the equations governing the motion of the point mass in x and y.

b. Under what conditions is this approximated by a potential function $V(x, y) = mgh(x, y)$?

c. Assume that we have an $h(x, y)$ which is axisymmetric about $x = y = 0$. Can you find such an h that yields motions with closed orbits?

1.10.2 Derivative Constraints

Here we investigate velocity-dependent constraints that are "total time derivatives" of velocity independent constraints. The methods presented so far do not apply because the constraint is velocity-dependent.

Consider a velocity-dependent constraint $\psi = 0$. That ψ is a total time derivative means that there exists a velocity-independent function φ such that

$$\psi \circ \Gamma[q] = D(\varphi \circ \Gamma[q]). \tag{1.174}$$

That φ is velocity independent means $\partial_2 \varphi = 0$. As state functions the relationship between ψ and φ is

$$\psi = D_t \varphi = \partial_0 \varphi + \partial_1 \varphi \dot{Q}. \tag{1.175}$$

Given a ψ we can find φ by solving this linear partial differential equation. The solution is determined up to a constant, so $\psi = 0$ implies $\varphi = K$ for some constant K. On the other hand, if we knew $\varphi = K$ then $\psi = 0$ follows. Thus the velocity-dependent constraint $\psi = 0$ is equivalent to the velocity-independent constraint $\varphi = K$, and we know how to find Lagrange equations for such systems.

If L is a Lagrangian for the unconstrained problem, the Lagrange equations with the constraint $\varphi = K$ are

$$(\mathsf{E}[L] + \lambda\ \mathsf{E}[\varphi]) \circ \Gamma[q] = 0, \tag{1.176}$$

where λ is a function of time that will be eliminated during the solution process. The constant K does not affect the Lagrange equations. The function φ is velocity-independent $\partial_2\varphi = 0$, so the Lagrange equations become

$$(\mathsf{E}[L] - \lambda\partial_1\varphi) \circ \Gamma[q] = 0. \tag{1.177}$$

From equation (1.175) we see that

$$\partial_1\varphi = \partial_2\psi, \tag{1.178}$$

so the Lagrange equations with the constraint $\psi = 0$ are

$$\mathsf{E}[L] \circ \Gamma[q] = \lambda\partial_2\psi \circ \Gamma[q]. \tag{1.179}$$

The important feature is that we can write the Lagrange equations directly in terms of ψ without having to produce the integral φ. Of course the validity of these Lagrange equations depends on the existence of the integral φ.

It turns out that the augmented Lagrangian trick also works here. These Lagrange equations are given if we augment the Lagrangian with the constraint ψ multiplied by a function of time λ':

$$L' = L + \lambda'\psi. \tag{1.180}$$

The Lagrange equations for L' turn out to be

$$\mathsf{E}[L] \circ \Gamma[q] = -D\lambda'\partial_2\psi \circ \Gamma[q], \tag{1.181}$$

which, with the identification $\lambda = -D\lambda'$, are the same as Lagrange equations (1.179).

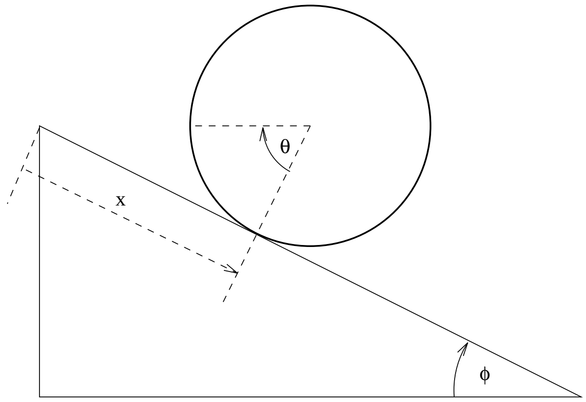

Figure 1.10 A massive hoop rolling, without slipping, down an inclined plane.

Sometimes a problem is naturally formulated in terms of velocity-dependent constraints. The formalism we have developed will handle any velocity-dependent constraint that can be written in terms of the derivative of a coordinate constraint. Such a constraint is called an *integrable constraint*. Any system for which the constraints can be put in the form of a coordinate constraint, or are already in that form, is called a *holonomic system*.

Exercise 1.34:

Show that the augmented Lagrangian (1.180) does lead to the Lagrange equations (1.181), taking into account the fact that ψ is a total time derivative of φ.

Goldstein's Hoop

Here we consider a problem for which the constraint can be represented as a time derivative of a coordinate constraint: a hoop of mass M rolling, without slipping, down a (one-dimensional) inclined plane (see figure 1.10).[75]

We will formulate this problem in terms of the two coordinates θ, the rotation of an arbitrary point on the hoop from an arbitrary reference direction, and x, the linear progress down the inclined plane. The constraint is that the hoop does not slip. Thus a

[75]This example appears in [10] pages 49–51,

change in θ is exactly reflected in a change in x; the constraint function is:

$$\psi(t; x, \theta; \dot{x}, \dot{\theta}) = R\dot{\theta} - \dot{x} \tag{1.182}$$

This constraint is phrased as a relation among generalized velocities, but it could be integrated to get $x = R\theta + c$. We may form our augmented Lagrangian with either the integrated constraint or its derivative.

The kinetic energy has two parts, the energy of rotation of the hoop and the energy of the motion of its center of mass.[76] The potential energy of the hoop decreases as the height decreases. Thus we may write the augmented Lagrangian:

$$\begin{aligned} &L(t; x, \theta, \lambda; \dot{x}, \dot{\theta}, \dot{\lambda}) \\ &\quad = \tfrac{1}{2}MR^2\dot{\theta}^2 + \tfrac{1}{2}M\dot{x}^2 + Mgx\sin\varphi + \lambda(R\dot{\theta} - \dot{x}) \end{aligned} \tag{1.183}$$

Lagrange's equations are

$$MD^2x - D\lambda = Mg\sin\varphi \tag{1.184}$$

$$MR^2D^2\theta + R\, D\lambda = 0 \tag{1.185}$$

$$R\, D\theta - Dx = 0. \tag{1.186}$$

And by differentiation of the third Lagrange equation we obtain,

$$D^2x = RD^2\theta. \tag{1.187}$$

By combining these equations we can solve for the dynamical quantities of interest. For this case of a rolling hoop the linear acceleration

$$D^2x = \tfrac{1}{2}g\sin\varphi \tag{1.188}$$

is just half of what it would have been if the mass had just slid down a frictionless plane without rotating. Note that for this hoop D^2x is independent of both M and R. We see from the Lagrange

[76] We will see in Chapter 2 how to compute the kinetic energy of rotation, but for now the answer is $\frac{1}{2}MR^2\dot{\theta}^2$

equations that $D\lambda$ can be interpreted as the friction force involved in enforcing the constraint. The frictional force of constraint is

$$D\lambda = \tfrac{1}{2} M g \sin\varphi \tag{1.189}$$

and the angular acceleration is

$$D^2\theta = \tfrac{1}{2}\tfrac{g}{R} \sin\varphi. \tag{1.190}$$

1.10.3 Non-Holonomic Systems

Systems with constraints that are not integrable are termed *non-holonomic systems*. A constraint is not integrable if it cannot be written in terms of an equivalent coordinate constraint. An example of a non-holonomic system is a ball rolling without slipping in a bowl. As the ball rolls it must turn so that the surface of the ball does not move relative to the bowl at the point of contact. This looks like it might establish a relation between the location of the ball in the bowl and the orientation of the ball, but it doesn't. The ball may return to the same place in the bowl with different orientations depending on the intervening path the ball has taken. As a consequence the constraints may not be used to eliminate any coordinates.

What are the equations of motion governing non-holonomic systems? For the restricted set of systems with non-holonomic constraints that are linear in the velocities, it is widely reported[77] that the equations of motion are the following. Let ψ have the form

$$\psi(t, q, v) = G_1(t, q)v + G_2(t, q), \tag{1.191}$$

a state function that is linear in the velocities. We assume ψ is not a total time derivative. If L is a Lagrangian for the unconstrained system, then the equations of motion are asserted to be

$$\mathsf{E}[L] \circ \Gamma[q] = \lambda G_1 \circ \Gamma[q] = \lambda \partial_2 \psi \circ \Gamma[q]. \tag{1.192}$$

Together with the constraint $\psi = 0$ the system is closed and the evolution of the system is determined. Note that these equations are identical to the Lagrange equations (1.179) for the case that ψ

[77] For some treatments of non-holonomic systems see, for example, Whittaker [24], Goldstein [10], Gantmakher [21], or Arnold *et al.* [8].

is a total time derivative, but here the derivation of those equations is no longer valid.

An essential step in the derivation of the Lagrange equations for coordinate constraints $\varphi = 0$ with $\partial_2\varphi = 0$ was to note that two conditions must be satisfied

$$(\mathsf{E}[L] \circ \Gamma[q])\eta = 0, \tag{1.193}$$

and

$$(\partial_1\varphi \circ \Gamma[q])\eta = 0. \tag{1.194}$$

Because $\mathsf{E}[L] \circ \Gamma[q]$ is orthogonal to η, and η is constrained to be orthogonal to $\partial_1\varphi \circ \Gamma[q]$ the two must be parallel at each moment:

$$\mathsf{E}[L] \circ \Gamma[q] = \lambda\partial_1\varphi \circ \Gamma[q]. \tag{1.195}$$

The Lagrange equations for derivative constraints were derived from this.

This derivation does not go through if the constraint function is velocity dependent. In this case, for a variation η to be consistent with the velocity-dependent constraint function ψ it must satisfy (see equation 1.148)

$$(\partial_1\psi \circ \Gamma[q])\eta + (\partial_2\psi \circ \Gamma[q])D\eta = 0. \tag{1.196}$$

We may no longer eliminate η by the same argument, because η is no longer orthogonal to $\partial_1\psi \circ \Gamma[q]$, and we cannot rewrite the constraint as a coordinate constraint because ψ is, by assumption, not integrable.

The following is the derivation of the non-holonomic equations from Arnold, et al. ([8]), translated into our notation. Define the "virtual velocities" ξ to be any velocity satisfying

$$(\partial_2\psi \circ \Gamma[q])\xi = 0. \tag{1.197}$$

The "principle of d'Alembert-Lagrange," according to Arnold, states that

$$(\mathsf{E}[L] \circ \Gamma[q])\xi = 0, \tag{1.198}$$

for any virtual velocity ξ. Because ξ is arbitrary except that it is required to be orthogonal to $\partial_2\psi \circ \Gamma[q]$ and any such ξ is orthogonal to $\mathsf{E}[L] \circ \Gamma[q]$, then $\partial_2\psi \circ \Gamma[q]$ must be parallel to $\mathsf{E}[L] \circ \Gamma[q]$. So

$$\mathsf{E}[L] \circ \Gamma[q] = \lambda(\partial_2\psi \circ \Gamma[q]), \tag{1.199}$$

which are the non-holonomic equations.

To convert the stationary action equations to the equations of Arnold we must do the following. To get from equation (1.193) to equation (1.198), we must replace η by ξ. However, to get from equation (1.196) to equation (1.197), we must set $\eta = 0$ and replace $D\eta$ by ξ. All "derivations" of the non-holonomic equations have similar identifications. It comes down to this: the non-holonomic equations do not follow from the action principle. They are something else. Whether they are correct or not depends on whether they agree with experiment.

For systems with coordinate constraints or derivative constraints we have found that the Lagrange equations can be derived from a Lagrangian that is augmented with the constraint. However, if the constraints are not integrable the Lagrange equations for the augmented Lagrangian are not the same as the non-holonomic system (equations 1.192).[78] Let L' be an augmented Lagrangian with non-integrable constraint ψ:

$$L'(t; q, \lambda; \dot{q}, \dot{\lambda}) = L(t, q, \dot{q}) + \lambda\psi(t, q, \dot{q}) \tag{1.200}$$

then the Lagrange equations associated with the coordinates are:

$$\begin{aligned} 0 &= \mathsf{E}[L] \circ \Gamma[q] \\ &\quad + D\lambda(\partial_2\psi) \circ \Gamma[q] + \lambda D((\partial_2\psi) \circ \Gamma[q]) - \lambda(\partial_1\psi) \circ \Gamma[q]. \end{aligned} \tag{1.201}$$

The Lagrange equation associated with λ is just the constraint equation

$$\psi \circ \Gamma[q] = 0. \tag{1.202}$$

An interesting feature of these equations is that they involve both λ and $D\lambda$. Thus the usual state variables q and Dq, with the constraint, are not sufficient to determine a full set of initial con-

[78] Arnold, et al. [8] call the variational mechanics with the constraints added to the Lagrangian *Vakonomic mechanics.*

ditions for the derived Lagrange equations, we need to specify an initial value for λ as well.

In general, for any particular physical system, equations (1.192) and (1.201) are not the same, and in fact they have different solutions. It is not apparent that either set of equations accurately models the physical system. The first approach to non-holonomic systems is not justified by extension of the arguments for the holonomic case and the other is not fully determined. Perhaps this is an indication that the models are inadequate; that more details of how the constraints are maintained need to be specified.

1.11 Summary of chapter 1

To analyze a mechanical system we construct an action function that gives us a way to distinguish realizable motions from other conceivable motions of the system. The action function is constructed so as to be stationary only on paths describing realizable motions, with respect to variations of the path. This is called the principle of stationary action. The principle of stationary action is a coordinate-independent specification of the realizable paths. For systems with or without constraints we may choose any system of coordinates that uniquely determines the configuration of the system.

For a large variety of mechanical systems actions are integrals of a function, called the Lagrangian, along the path. For many systems an appropriate Lagrangian is the difference of the kinetic energy and the potential energy of the system. The choice of a Lagrangian for a system is not unique.

For any system that we have a Lagrangian action we can formulate a system of ordinary differential equations, the Lagrange equations, that is satisfied by any realizable path. The method of deriving the Lagrange equations from the Lagrangian is independent of the coordinate system used to formulate the Lagrangian. One freedom we have in formulation is that the addition of a total time derivative to a Lagrangian for a system yields another Lagrangian that has the same Lagrange equations.

The Lagrange equations are a set of ordinary differential equations: there is a finite state that summarizes the history of the system and is sufficient to determine the future. There is an effective procedure for evolving the motion of the system from a state at an instant. For many systems the state is determined by the coordinates and the rate of change of the coordinates at an instant.

If there are continuous symmetries in a physical system there are conserved quantities associated with them. If the system can be formulated in such a way that the symmetries are manifest in missing coordinates in the Lagrangian then there are conserved momenta conjugate to those coordinates. If the Lagrangian is independent of time then there is a conserved energy.

1.12 Projects

Exercise 1.35: A numerical investigation

Consider a pendulum: a mass m supported on a massless rod of length l, in a uniform gravitational field. A Lagrangian for the pendulum is:

$$L(t, \theta, \dot{\theta}) = \frac{m}{2}(l\dot{\theta})^2 + mgl\cos\theta$$

For the pendulum, the period of the motion depends on the amplitude. We wish to find trajectories of the pendulum with a given frequency. Three methods of doing this present themselves: (1) solution by the principle of least action, (2) numerical integration of Lagrange's equation, and (3) analytic solution (which requires some exposure to elliptic functions). We will carry out all three, and compare the solution trajectories.

To be specific, consider the parameters $m = 1kg$, $l = 1m$, $g = 9.8ms^{-2}$. The frequency of small amplitude oscillations is $\omega_0 = \sqrt{g/l}$. Let's find the non-trivial solution that has the frequency $\omega_1 = \frac{4}{5}\omega_0$.

a. The angle is periodic in time, so a Fourier series representation is appropriate. We can choose the origin of time so that a zero crossing of the angle is at time zero. Since the potential is even in the angle, the angle is an odd function of time. Thus we need only a sine series. Since the angle returns to zero after one-half period the angle is an odd function of time about the midpoint. Thus only odd terms of the series are present:

$$\theta(t) = \sum_{n=1}^{m} A_n \sin((2n-1)\omega_1 t).$$

The amplitude of the trajectory is $A = \theta_{\max} = \sum_{n=1}^{\infty}(-1)^{n+1}A_n$.

Find approximations to the first few coefficients A_n by minimizing the action. You will have to write a program similar to the `find-path` procedure in section 1.4. Watch out: there is more than one trajectory that minimizes the action.

b. Write a program to numerically integrate Lagrange's equations for the trajectories of the pendulum. The trouble with using numerical integration to solve this problem is that we do not know how the frequency of the motion depends on the initial conditions. So we have to guess, and then gradually improve our guess. Define a function $\Omega(\dot\theta)$ that numerically computes the frequency of the motion as a function of the initial angular velocity (with $\theta = 0$). Find the trajectory by solving $\Omega(\dot\theta) = \omega$, for the initial angular velocity of the desired trajectory. Methods of solving this equation include successive bisection, minimizing the squared residual, etc. – choose one.

c. Now let's formulate the analytic solution for the frequency as a function of amplitude. The period of the motion is simply

$$T = 4\int_0^{T/4} dt = 4\int_0^A \frac{1}{\dot\theta} d\theta.$$

Using the energy, solve for $\dot\theta$ in terms of the amplitude A and θ to write the required integral explicitly. This integral can be written in terms of elliptic functions, but in a sense this does not solve the problem – we still have to compute the elliptic functions. Let's avoid this excursion into elliptic functions and just do the integral numerically using the procedure `definite-integral`. We still have the problem that we can specify the amplitude A and get the frequency but to solve our problem we need to solve the inverse problem, but that can be done as in part **b**.

Exercise 1.36: Double Pendulum Behavior

Consider the ideal double pendulum show in figure 1.11.

a. Formulate a Lagrangian to describe the dynamics. Derive the equations of motion in terms of the given angles θ_1 and θ_2. Put the equations into a form appropriate for numerical integration.
Assume the following system parameters:

$$\begin{aligned} g &= 9.8\ \frac{\mathrm{m}}{\mathrm{sec}^2} \\ l_1 &= 1.0\ \mathrm{m} \\ l_2 &= 0.9\ \mathrm{m} \\ m_1 &= 1.0\ \mathrm{kg} \\ m_2 &= 3.0\ \mathrm{kg} \end{aligned}$$

b. Prepare graphs showing the behavior of each angle as a function of time when the pendulums are started with the initial conditions:

$$\begin{aligned} \theta_1(0) &= \frac{\pi}{2}\ \text{radian} \\ \theta_2(0) &= \pi\ \text{radian} \end{aligned}$$

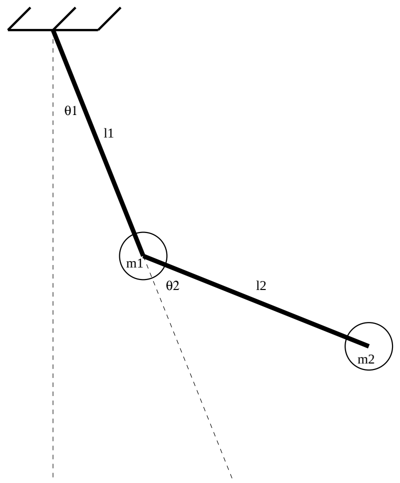

Figure 1.11 The double pendulum is pinned in two joints so that its members are free to move in a plane.

$$\dot{\theta}_1(0) = 0\ \frac{\text{radian}}{\text{sec}}$$
$$\dot{\theta}_2(0) = 0\ \frac{\text{radian}}{\text{sec}}$$

Make the graphs extend to 50 seconds. Save the state points at .125 second intervals in a list.

c. Make a graph of the behavior of the energy of your system as a function of time. The energy should be conserved. How good is the conservation you obtained?

d. Repeat the experiment of part **b** with the m_2 bob 10^{-10} m higher than before. Form the list of squared differences of the distances between the m_2 bobs in the two experiments, and plot the log of that against time. What do you see?

e. Repeat the previous comparison, but this time with the initial conditions:

$$\theta_1(0) = \frac{\pi}{2}\ \text{radian}$$
$$\theta_2(0) = 0\ \text{radian}$$
$$\dot{\theta}_1(0) = 0\ \frac{\text{radian}}{\text{sec}}$$
$$\dot{\theta}_2(0) = 0\ \frac{\text{radian}}{\text{sec}}$$

What do you see here?

2
Rigid Bodies

The motion of rigid bodies presents many surprising phenomena.

Consider the motion of a top. A top is usually thought of as an axisymmetric body, subject to gravity, with a point on the axis of symmetry that is fixed in space. The top is spun, and in general executes some complicated motion. We observe that the top usually settles down into an unusual motion in which the axis of the top slowly precesses about the vertical, apparently moving perpendicular to the direction in which gravity is attempting to accelerate it.

Consider the motion of a book thrown into the air.[1] Books have three main axes. Idealized as a brick with rectangular faces, the three axes are the lines through the centers of opposite faces. Try spinning the book about each axis. The motion of the book spun about the longest and the shortest axis is a simple regular rotation, perhaps with a little wobble depending on how carefully it is thrown. The motion of the book spun about the intermediate axis is qualitatively different: however carefully the book is spun about the intermediate axis the book tumbles.

The rotation of the Moon is peculiar in that the Moon always presents the same face to the Earth, indicating that the rotational period and the orbit period are the same. Considering that the orbit of the Moon is constantly changing because of interactions with the Sun and other planets, and therefore the orbital period of the Moon is constantly undergoing small variations, we might expect that the face of the Moon that we see would slowly change, but it does not. What is special about the face that is presented to us?

A rigid body may be thought of as a large number of constituent particles with rigid constraints among them. Thus the dynamical principles governing the motion of rigid bodies are the same as those governing the motion of any other system of particles with rigid constraints. What is new here is that the number of consituent particles is very large and we need to develop new tools to handle them effectively.

---

[1] We put a rubber band around the book so that it does not open.

We have found that a Lagrangian for a system with rigid constraints can be written as the difference of the kinetic and potential energies. The kinetic and potential energies are naturally expressed in terms of the positions and velocities of the constituent particles. To write the Lagrangian in terms of the generalized coordinates and velocities we must specify functions that relate the generalized coordinates to the positions of the constituent particles. In the systems with rigid constraints considered up to now these functions were explicitly given for each of the constituent particles and individually included in the derivation of the Lagrangian. For a rigid body there are too many consituent particles to handle each one of them in this way. We need to find means of expressing the kinetic and potential energies of rigid bodies in terms of the generalized coordinates and velocities, without going through the particle-by-particle details.

The strategy is to first rewrite the kinetic and potential energies in terms of quantities that characterize essential aspects of the distribution of mass in the body and the state of motion of the body. Only later do we introduce generalized coordinates. For the kinetic energy, it turns out a small number of parameters completely specify the state of motion and the relevant aspects of the distribution of mass in the body. For the potential energy, we find that for some specific problems the potential energy can be represented with a small number of parameters, but in general we have to make approximations to obtain a representation with a manageable number of parameters.

2.1 Rotational Kinetic Energy

We consider a rigid body to be made up of a large number of constituent particles with mass m_α, position $\vec{x}_\alpha$, and velocities $\dot{\vec{x}}_\alpha$, with rigid positional constraints among them. The kinetic energy is

$$\sum_\alpha \tfrac{1}{2} m_\alpha \dot{\vec{x}}_\alpha \cdot \dot{\vec{x}}_\alpha. \tag{2.1}$$

It turns out that the kinetic energy of a rigid body can be separated into two pieces: a kinetic energy of translation and a kinetic energy of rotation. Let's see how this comes about.

The configuration of a rigid body is fully specified given the location of any point in the body and the orientation of the body. This suggests that it would be useful to decompose the position vectors for the constituent particles as the sum of the vector $\vec{X}$ to some reference position in the body and the vector $\vec{\xi}_\alpha$ from the reference position to the particular constituent element with index α:

$$\vec{x}_\alpha = \vec{X} + \vec{\xi}_\alpha. \tag{2.2}$$

Along paths, the velocities are related by

$$\dot{\vec{x}}_\alpha = \dot{\vec{X}} + \dot{\vec{\xi}}_\alpha. \tag{2.3}$$

So in terms of $\dot{\vec{X}}$ and $\dot{\vec{\xi}}_\alpha$ the kinetic energy is

$$\begin{aligned}\sum_\alpha \tfrac{1}{2} m_\alpha \left(\dot{\vec{X}} + \dot{\vec{\xi}}_\alpha\right) \cdot \left(\dot{\vec{X}} + \dot{\vec{\xi}}_\alpha\right) \\ = \sum_\alpha \tfrac{1}{2} m_\alpha \left(\dot{\vec{X}} \cdot \dot{\vec{X}} + 2\dot{\vec{X}} \cdot \dot{\vec{\xi}}_\alpha + \dot{\vec{\xi}}_\alpha \cdot \dot{\vec{\xi}}_\alpha\right).\end{aligned} \tag{2.4}$$

If we select the reference position in the body to be its *center of mass*,

$$\vec{X} = \frac{1}{M} \sum_\alpha m_\alpha \vec{x}_\alpha, \tag{2.5}$$

where $M = \sum_\alpha m_\alpha$ is the total mass of the body, then

$$\sum_\alpha m_\alpha \vec{\xi}_\alpha = \sum_\alpha m_\alpha (\vec{x}_\alpha - \vec{X}) = 0. \tag{2.6}$$

So along paths the relative velocities satisfy

$$\sum_\alpha m_\alpha \dot{\vec{\xi}}_\alpha = 0. \tag{2.7}$$

The kinetic energy is then

$$\sum_\alpha \tfrac{1}{2} m_\alpha \dot{\vec{X}} \cdot \dot{\vec{X}} + \textstyle\sum_\alpha \tfrac{1}{2} m_\alpha \dot{\vec{\xi}}_\alpha \cdot \dot{\vec{\xi}}_\alpha. \tag{2.8}$$

The kinetic energy is the sum of the kinetic energy of the motion of the total mass at the center of mass

$$\tfrac{1}{2}M\dot{\vec{X}} \cdot \dot{\vec{X}}, \tag{2.9}$$

and the kinetic energy of rotation about the center of mass

$$\sum_{\alpha} \tfrac{1}{2}m_{\alpha}\dot{\vec{\xi}}_{\alpha} \cdot \dot{\vec{\xi}}_{\alpha}. \tag{2.10}$$

Written in terms of appropriate generalized coordinates the kinetic energy is a Lagrangian for a free rigid body. If we choose generalized coordinates so that the center of mass position is entirely specified by some of them and the orientation is entirely specified by others, then the Lagrange equations for a free rigid body will decouple into two groups of equations, one concerned with the motion of the center of mass and one concerned with the orientation.

Such a separation might occur in other problems, such as a rigid body moving in a uniform gravitational field, but in general, potential energies cannot be separated as the kinetic energy separates. So the motion of the center of mass and the rotational motion are usually coupled through the potential. Even in these cases, it is usually an advantage to choose generalized coordinates that separately specify the position of the center of mass and the orientation.

2.2 Kinematics of Rotation

The motion of a rigid body about a center of rotation, a reference position that is fixed with respect to the body, is characterized at each moment by a rotation axis and a rate of rotation. Let's elaborate.

We can get from any orientation of a body to any other orientation of the body by a rotation of the body. That this is true is called Euler's theorem.[2] We know that rotations have the property that they do not commute: the composition of successive rotations in general depends on the order of operation. Rotating a book about the $\hat{x}$ axis and then about the $\hat{z}$ axis puts the book

[2] For an elementary geometric proof of Euler's theorem see Whittaker [24].

in a different orientation than rotating the book about the $\hat{z}$ axis and then about the $\hat{x}$ axis. Nevertheless, Euler's theorem states that however many rotations have been composed to reach a given orientation, the orientation could have been reached with a single rotation. Try it! We take a book, rotate it this way, then that, and then some other way — then find the rotation that does the job in one step. So a rotation can be specified by an axis of rotation and the angular amount of the rotation.

If the orientation of a body evolves over some interval of time then the orientation at the beginning and the end of the interval can be connected by a single rotation. In the limit that the duration of the interval goes to zero the rotation axis approaches a unique instantaneous rotation axis. And in this limit the ratio of the angle of rotation and the duration of the interval approaches the instantaneous rate of rotation. We represent this instantaneous rotational motion by the *angular velocity vector* $\vec{\omega}$, which points in the direction of the rotation axis (with the right-hand rule giving the direction of rotation about the axis) and has a magnitude equal to the rate of rotation.

If the angular velocity vector for a body is $\vec{\omega}$ then the velocities of the constituent particles are perpendicular to the vectors to the constituent particles and proportional to the rate of rotation of the body and the distance of the constituent particle from the instantaneous rotation axis:

$$\dot{\vec{\xi}}_\alpha = \vec{\omega} \times \vec{\xi}_\alpha. \tag{2.11}$$

Isn't it interesting that we have found a concise way of specifying how the orientation of the body is changing, even though we have not yet described a way to specify the orientation itself.

2.3 Moments of Inertia

The rotational kinetic energy is the sum of the kinetic energy of each of the constituents of the rigid body. We can rewrite the rotational kinetic energy in terms of the angular velocity vector and certain aggregate quantities determined by the distribution of mass in the rigid body.

Substituting our representation of the relative velocity vectors into the rotational kinetic energy we obtain

$$\sum_\alpha \tfrac{1}{2} m_\alpha \dot{\vec{\xi}}_\alpha \cdot \dot{\vec{\xi}}_\alpha = \sum_\alpha \tfrac{1}{2} m_\alpha \left(\vec{\omega} \times \vec{\xi}_\alpha\right) \cdot \left(\vec{\omega} \times \vec{\xi}_\alpha\right). \tag{2.12}$$

We introduce an arbitrary rectangular coordinate system with origin at the center of rotation and with basis vectors $\hat{e}_1$, $\hat{e}_2$, and $\hat{e}_3$, with the property that $\hat{e}_1 \times \hat{e}_2 = \hat{e}_3$. The components of $\vec{\omega}$ on this coordinate system are ω^1, ω^2, and ω^3. Rewriting $\vec{\omega}$ in terms of its components, the rotational kinetic energy becomes

$$\begin{aligned}
&\sum_\alpha \tfrac{1}{2} m_\alpha \left(\left(\textstyle\sum_i \hat{e}_i \omega^i\right) \times \vec{\xi}_\alpha\right) \cdot \left(\left(\textstyle\sum_j \hat{e}_j \omega^j\right) \times \vec{\xi}_\alpha\right) \\
&\qquad = \tfrac{1}{2} \textstyle\sum_{ij} \omega^i \omega^j \sum_\alpha m_\alpha \left(\hat{e}_i \times \vec{\xi}_\alpha\right) \cdot \left(\hat{e}_j \times \vec{\xi}_\alpha\right) \\
&\qquad = \tfrac{1}{2} \textstyle\sum_{ij} \omega^i \omega^j I_{ij},
\end{aligned} \tag{2.13}$$

with

$$I_{ij} = \sum_\alpha m_\alpha \left(\hat{e}_i \times \vec{\xi}_\alpha\right) \cdot \left(\hat{e}_j \times \vec{\xi}_\alpha\right). \tag{2.14}$$

The quantities I_{ij} are the components of the *inertia tensor* with respect to the chosen coordinate system. Note what a remarkable form the kinetic energy has taken. All we have done is interchange the order of summations, but now the kinetic energy is written as a sum of products of components of the angular velocity vector, which completely specifies how the orientation of the body is changing, and the quantity I_{ij} which depends solely on the distribution of mass in the body relative to the chosen coordinate system.

We will deduce a number of properties of the inertia tensor. First, we find a somewhat simpler expression for it. The components of the vector $\vec{\xi}_\alpha$ are $(\xi_\alpha, \eta_\alpha, \zeta_\alpha)$.[3] Rewriting $\vec{\xi}_\alpha$ as a sum over its components, and simplifying the elementary vector prod-

[3]Here we avoid the more consistent notation $(\xi^0_\alpha, \xi^1_\alpha, \xi^2_\alpha)$ for the components of $\vec{\xi}_\alpha$ because it is awkward to write expressions involving powers of the components written this way.

ucts of basis vectors, the components of the inertia tensor can be arranged in the *inertia matrix*

$$\mathbf{I} = \begin{bmatrix} \sum_\alpha m_\alpha(\eta_\alpha^2 + \zeta_\alpha^2) & -\sum_\alpha m_\alpha \xi_\alpha \eta_\alpha & -\sum_\alpha m_\alpha \xi_\alpha \zeta_\alpha \\ -\sum_\alpha m_\alpha \eta_\alpha \xi_\alpha & \sum_\alpha m_\alpha(\xi_\alpha^2 + \zeta_\alpha^2) & -\sum_\alpha m_\alpha \eta_\alpha \zeta_\alpha \\ -\sum_\alpha m_\alpha \zeta_\alpha \xi_\alpha & -\sum_\alpha m_\alpha \zeta_\alpha \eta_\alpha & \sum_\alpha m_\alpha(\xi_\alpha^2 + \eta_\alpha^2) \end{bmatrix}. \tag{2.15}$$

The inertia tensor has real components and is symmetric: $I_{jk} = I_{kj}$.

We define the *moment of inertia* I about a line by

$$I = \sum_\alpha m_\alpha (\xi_\alpha^\perp)^2, \tag{2.16}$$

where $\xi_\alpha^\perp$ is the perpendicular distance from the line to the constituent with index α. The diagonal components of the inertia tensor I_{ii} are recognized as the moments of inertia about the lines coinciding with the coordinate axes $\hat{e}_i$. The off-diagonal components of the inertia tensor are called *products of inertia*.

The rotational kinetic energy of a body depends on the distribution of mass of the body solely through the inertia tensor. Remarkably, the inertia tensor involves only second order moments of the mass distribution with respect to the center of mass. We might have expected the kinetic energy to depend in a complicated way on all the moments of the mass distribution, interwoven in some complicated way with the components of the angular velocity vector, but this is not the case. This fact has a remarkable consequence: for the motion of a free rigid body the detailed shape of the body does not matter. If a book and a banana have the same inertia tensor, that is, the same second order mass moments, then if they are thrown in the same way the subsequent motion will be the same, however complicated that motion is. The fact that the book has corners and the banana has a stem do not affect the motion except for their contributions to the inertia tensor. In general, the potential energy of an extended body is not so simple and does indeed depend on all moments of the mass distribution, but for the kinetic energy the second moments are all that matter!

Exercise 2.1: Rotational Kinetic Energy

An interesting alternate form for the rotational kinetic energy can be found by decomposing $\vec{\xi}_\alpha$ into components parallel and perpendicular to the rotation axis $\hat{\omega}$. Show that the rotational kinetic energy can also be written

$$T_{\mathrm{R}} = \tfrac{1}{2} I \omega^2, \tag{2.17}$$

where I is the moment of inertia about the line through the center of mass with direction $\hat{\omega}$, and ω is the instantaneous rate of rotation.

Exercise 2.2: Steiner's Theorem

Let I be the moment of inertia of a body with respect to some given line through the center of mass. Show that the moment of inertia I' with respect to a second line parallel to the first is

$$I' = I + MR^2 \tag{2.18}$$

where M is the total mass of the body and R is the distance between the lines.

Exercise 2.3: Some Useful Moments of Inertia

Show that the moments of inertia of the following objects are as given:

a. The moment of inertia of a sphere of uniform density with mass M and radius R about any line through the center is $\frac{2}{5}MR^2$.

b. The moment of inertia of a spherical shell with mass M and radius R about any line through the center is $\frac{2}{3}MR^2$.

c. The moment of inertia of a cylinder of uniform density with mass M and radius R about the axis of the cylinder is $\frac{1}{2}MR^2$.

c. The moment of inertia of a thin rod of uniform density per unit length with mass M and length L about an axis perpendicular to the rod through the center of mass is $\frac{1}{12}ML^2$.

Exercise 2.4: Jupiter

a. The density of a planet increases toward the center. Provide an argument that the moment of inertia is less than that of a sphere of uniform density of the same mass and radius.

b. The density as a function of radius inside Jupiter is well approximated by

$$\rho(r) = \frac{M}{R^3} \frac{\sin(\pi r/R)}{4r/R},$$

where M is the mass and R is the radius of Jupiter. Find the moment of inertia of Jupiter in terms of M and R.

2.4 Inertia Tensor

The representation of the rotational kinetic energy in terms of the inertia tensor was derived with the help of a rectangular coordinate system with basis vectors $\hat{e}_i$. There was nothing special about this particular rectangular basis. So, the kinetic energy must have the same form in any rectangular coordinate system. We can use this fact to derive how the inertia tensor changes if the body or the coordinate system is rotated.

Let's talk a bit about *active* and *passive* rotations. The rotation of the vector $\vec{x}$ by the rotation R produces a new vector $\vec{x}' = R\vec{x}$. We may write $\vec{x}$ in terms of its components with respect to some arbitrary rectangular coordinate system with orthonormal basis vectors $\hat{e}_i$: $\vec{x} = x^1\hat{e}_1 + x^2\hat{e}_2 + x^3\hat{e}_3$. Let $\mathbf{x}$ indicate the column matrix of components x^1, x^2, and x^3 of $\vec{x}$, and $\mathbf{R}$ be the matrix representation of R with respect to the same basis. In these terms rotation can be written $\mathbf{x}' = \mathbf{R}\mathbf{x}$. The rotation matrix $\mathbf{R}$ is a real orthogonal matrix.[4] A rotation that carries vectors to new vectors is called an *active* rotation.

Alternately, we can rotate the coordinate system by rotating the basis vectors, but leave other vectors that might be represented in terms of them unchanged. If a vector is unchanged but the basis vectors are rotated then the components of the vector on the rotated basis vectors are not the same as the components on the original basis vectors. Denote the rotated basis vectors by $\hat{e}'_i = R\hat{e}_i$. The component of a vector along a basis vector is the dot product of the vector with the basis vector. So the components of the vector $\vec{x}$ along the rotated basis $\hat{e}'_i$ are $(x')^i = \vec{x} \cdot \hat{e}'_i = \vec{x} \cdot (R\hat{e}_i) = (R^{-1}\vec{x}) \cdot \hat{e}_i$.[5] So the components with respect to the rotated basis elements are the same as the components of the rotated vector $R^{-1}\vec{x}$ with respect to the original basis. In terms of components, if the vector $\vec{x}$ has components $\mathbf{x}$ with respect to the original basis vectors $\hat{e}_i$, then the components $\mathbf{x}'$ of the same vector with respect to the rotated basis vectors $\hat{e}'_i$ are $\mathbf{x}' = \mathbf{R}^{-1}\mathbf{x}$, or equivalently $\mathbf{x} = \mathbf{R}\mathbf{x}'$. A rotation that actively rotates the basis vectors, leaving other vectors unchanged, is called a *passive*

[4] An orthogonal matrix $\mathbf{R}$ satisfies $\mathbf{R}^{\mathsf{T}} = \mathbf{R}^{-1}$ and $\det \mathbf{R} = 1$.

[5] The last equality follows from the fact that the rotation of two vectors preserves the dot product: $\vec{x} \cdot \vec{y} = (R\vec{x}) \cdot (R\vec{y})$, or $(R^{-1}\vec{x}) \cdot \vec{y} = \vec{x} \cdot (R\vec{y})$.

rotation. For a passive rotation the components of a fixed vector change as if the vector was actively rotated by the inverse rotation.

With respect to the rectangular basis $\hat{e}_i$ the rotational kinetic energy is written

$$\tfrac{1}{2}\sum_{ij}\omega^i\omega^j I_{ij}. \tag{2.19}$$

In terms of matrix representations, the kinetic energy is

$$\tfrac{1}{2}\boldsymbol{\omega}^{\mathrm{T}}\mathbf{I}\boldsymbol{\omega}, \tag{2.20}$$

where $\boldsymbol{\omega}$ is the column of components representing $\vec{\omega}$.[6] If we rotate the coordinate system by the passive rotation R about the center of rotation, the new basis vectors are $\hat{e}'_i = R\hat{e}_i$. The components $\boldsymbol{\omega}'$ of the vector $\vec{\omega}$ with respect to the rotated coordinate system satisfy

$$\boldsymbol{\omega} = \mathbf{R}\boldsymbol{\omega}' \tag{2.21}$$

where $\mathbf{R}$ is the matrix representation of R. The kinetic energy is

$$\tfrac{1}{2}(\boldsymbol{\omega}')^{\mathrm{T}}\mathbf{R}^{\mathrm{T}}\mathbf{I}\mathbf{R}\boldsymbol{\omega}'. \tag{2.22}$$

However, if we had started with the basis $\hat{e}'_i$, we would have written the kinetic energy directly as

$$\tfrac{1}{2}(\boldsymbol{\omega}')^{\mathrm{T}}\mathbf{I}'\boldsymbol{\omega}', \tag{2.23}$$

where the components are taken with respect to the $\hat{e}'_i$ basis. Comparing the two expressions, we see that

$$\mathbf{I}' = \mathbf{R}^{\mathrm{T}}\mathbf{I}\mathbf{R}. \tag{2.24}$$

Thus the inertia matrix transforms by a similarity transformation.[7]

---

[6] We take a 1-by-1 matrix as a number.

[7] That the inertia tensor transforms in this manner could have been deduced from its definition (2.14). However, it seems that this argument, based on the coordinate-system independence of the kinetic energy, provides insight.

2.5 Principal Moments of Inertia

We can use the transformation properties of the inertia tensor (2.24) to show that there are special rectangular coordinate systems for which the inertia tensor I' is diagonal, that is, $I'_{ij} = 0$ for $i \neq j$. Let's assume that $\mathbf{I}'$ is diagonal and solve for the rotation matrix $\mathbf{R}$ that does the job. Multiplying both sides of (2.24) on the left by $\mathbf{R}$ we have

$$\mathbf{R}\mathbf{I}' = \mathbf{I}\mathbf{R}. \tag{2.25}$$

We can examine pieces of this matrix equation by multiplying on the right by a trivial column vector that picks out a particular column. So we multiply on the right by the column matrix representation $\mathbf{e}_i$ of each of the coordinate unit vectors $\hat{e}_i$. These column matrices have a one in the i^{th} row and zeroes otherwise. Using $\mathbf{e}'_i = \mathbf{R}\mathbf{e}_i$, we find

$$\mathbf{R}\mathbf{I}'\mathbf{e}_i = \mathbf{I}\mathbf{R}\mathbf{e}_i = \mathbf{I}\mathbf{e}'_i. \tag{2.26}$$

The matrix $\mathbf{I}'$ is diagonal so

$$\mathbf{R}\mathbf{I}'\mathbf{e}_i = \mathbf{R}\mathbf{e}_i I'_{ii} = I'_{ii}\mathbf{e}'_i. \tag{2.27}$$

So, from equations (2.26) and (2.27), we have

$$I'_{ii}\mathbf{e}'_i = \mathbf{I}\mathbf{e}'_i, \tag{2.28}$$

which we recognize as an equation for the eigenvalue I'_{ii} and $\mathbf{e}'_i$, the column matrix of components of the associated eigenvector.

From $\mathbf{e}'_i = \mathbf{R}\mathbf{e}_i$, we see that the $\mathbf{e}'_i$ are the columns of the rotation matrix $\mathbf{R}$. Now, rotation matrices are orthogonal, so $\mathbf{R}^{\mathsf{T}}\mathbf{R} = \mathbf{1}$; thus the columns of the rotation matrix must be orthonormal $(\mathbf{e}'_i)^{\mathsf{T}}\mathbf{e}'_j = \delta_{ij}$, which is one if $i = j$ and zero otherwise. But the eigenvectors that are solutions of equation (2.28) are not necessarily even orthogonal. So we are not done yet.

If a matrix is real and symmetric then the eigenvalues are real. Furthermore, if the eigenvalues are distinct then the eigenvectors are orthogonal. However, if the eigenvalues are not distinct then the directions of the eigenvectors for the degenerate eigenvalues are not uniquely determined — but we have the freedom to choose particular $\mathbf{e}'_i$ which are orthogonal.[8] The linearity of equation (2.28) implies the $\mathbf{e}'_i$ can be normalized. Thus whether or not the eigenvalues are distinct we can obtain an orthonormal set of $\mathbf{e}_i$. This is enough to reconstruct a rotation matrix $\mathbf{R}$ that does the job we asked of it: to rotate the coordinate system to a configuration such that the inertia tensor is diagonal. If the eigenvalues are not distinct, the rotation matrix $\mathbf{R}$ is not uniquely defined — there is more than one rotation matrix $\mathbf{R}$ that does the job.

The eigenvectors and eigenvalues are determined by the requirement that the inertia tensor be diagonal with respect to the rotated coordinate system. Thus the rotated coordinate system has a special orientation with respect to the body. The basis vectors $\hat{e}'_i$ therefore actually point along particular directions in the body. We define the axes in the body through the center of mass with these directions to be the *principal axes*. With respect to the coordinate system defined by $\hat{e}'_i$ the inertia tensor is diagonal, by construction, with the eigenvalues I'_{ii} on the diagonal. Thus the moments of inertia about the principal axes are the eigenvalues I'_{ii}. We call the moments of inertia about the principal axes the *principal moments of inertia*.

For convenience, we often label the principal moments of inertia according to their size: $A \leq B \leq C$, with principal axis unit vectors $\hat{a}$, $\hat{b}$, $\hat{c}$, respectively. The positive direction along the principal axes can be chosen so that $\hat{a}$, $\hat{b}$, $\hat{c}$ form a right handed rectangular coordinate basis.

Let $\mathbf{x}$ represent the matrix of components of a vector $\vec{x}$ with respect to the basis vectors $\hat{e}_i$. Recall that the components $\mathbf{x}'$ of a vector $\vec{x}$ with respect to the principal axis unit vectors $\hat{e}'_i$ satisfy

$$\mathbf{x}' = \mathbf{R}^{\mathsf{T}}\mathbf{x}. \tag{2.29}$$

This makes sense because the columns of $\mathbf{R}$ are the components of $\mathbf{e}'_i$. Multiplying the components of $\vec{x}$ by the transpose of $\mathbf{R}$ is taking the dot product of each $\hat{e}'_i$ with $\vec{x}$ producing the components. The components of a vector on the principal axis basis are sometimes called the *body components* of the vector.

---

[8]If two eigenvalues are not distinct then linear combinations of the associated eigenvectors are eigenvectors. This gives us the freedom to find linear combinations of the eigenvalues which are orthonormal.

Now let's rewrite the kinetic energy in terms of the principal moments of inertia. If we choose our rectangular coordinate system so that it coincides with the principal axes then the calculation is simple. Let the components of the angular velocity vector on the principal axes be $(\omega^a, \omega^b, \omega^c)$. Then, keeping in mind that the inertia tensor is diagonal with respect to the principal axis basis, the kinetic energy is just

$$T_{\mathrm{R}} = \tfrac{1}{2}\left[A(\omega^a)^2 + B(\omega^b)^2 + C(\omega^c)^2\right]. \tag{2.30}$$

Exercise 2.5: A Constraint on the Moments of Inertia

Show that the sum of any two of the principal moments of inertia is greater than the third principal moment.

Exercise 2.6: Principal Moments of Inertia

For each of the configurations described below find the principal moments of inertia with respect to the center of mass; find the corresponding principal axes.

a. A regular tetrahedron consisting of four equal point masses tied together with rigid massless wire.

b. A cube of uniform density.

c. Five equal point masses rigidly connected by massless stuff. The point masses are at the rectangular coordinates:

$(-1, 0, 0), (1, 0, 0), (1, 1, 0), (0, 0, 0), (0, 0, 1)$

Exercise 2.7: This Book

Measure this book. You will admit that it is pretty dense. Don't worry, you will get to throw it later. Show that the principal axes are the lines connecting the centers of opposite faces of the idealized brick approximating the book. Compute the corresponding principal moments of inertia.

2.6 Representation of the Angular Velocity Vector

We can specify the orientation of a body by specifying the rotation that takes the body to this orientation from some reference orientation. As the body moves the rotation that does this changes. The angular velocity vector can be written in terms of this changing rotation along a path.

Let q be the coordinate path that we will use to describe the motion of the body. Let $\mathsf{M}(q(t))$ be the rotation that takes the

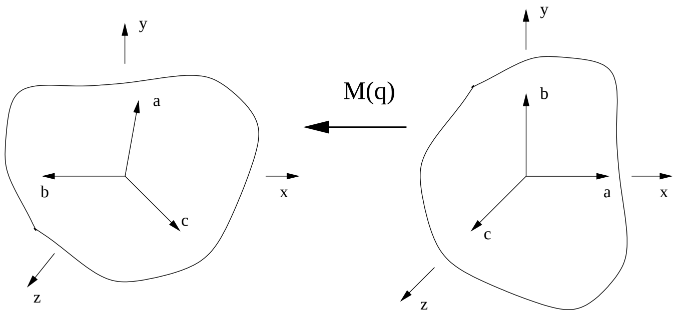

Figure 2.1 The rotation $\mathsf{M}(q)$ rotates the body from a reference orientation in which the principal axes are aligned with the basis $\hat{e}_i$ (labeled by x, y, and z here) to the orientation specified by q.

body from the reference orientation to the orientation specified by $q(t)$ (see Figure 2.1). Let $\vec{\xi}_\alpha(t)$ be the vector to some constituent with the body in the orientation specified by $q(t)$, and let $\vec{\xi'}_\alpha$ be the vector to the same constituent with the body in the reference orientation. Then

$$\vec{\xi}_\alpha(t) = \mathsf{M}(q(t))\vec{\xi'}_\alpha. \tag{2.31}$$

The constituent vectors $\vec{\xi'}_\alpha$ do not depend on the configuration, because they are the vectors to the positions of the constituents with the body in a fixed reference orientation.

We have already found an expression for the kinetic energy in terms of the angular velocity vector and the inertia tensor. Here we do this a different way. To compute the kinetic energy we accumulate the contributions from all of the mass elements. The positions of the constituent particles, at a given time t, are

$$\vec{\xi}_\alpha(t) = \mathsf{M}(q(t))\vec{\xi'}_\alpha = M(t)\vec{\xi'}_\alpha, \tag{2.32}$$

where $M = \mathsf{M} \circ q$. The velocity is the time derivative

$$D\vec{\xi}_\alpha(t) = DM(t)\vec{\xi'}_\alpha. \tag{2.33}$$

Using equation (2.32) we can write

$$D\vec{\xi}_\alpha(t) = DM(t)(M(t))^{-1}\vec{\xi}_\alpha(t). \tag{2.34}$$

Recall that the velocity results from a rotation, and that the velocities are (see equation 2.11)

$$D\vec{\xi}_\alpha(t) = \vec{\omega}(t) \times \vec{\xi}_\alpha(t). \tag{2.35}$$

Thus we can identify the operator $\vec{\omega}(t)\times$ with $DM(t)(M(t))^{-1}$ To form the kinetic energy we need to extract $\vec{\omega}(t)$ from this.

If a vector $\vec{u}$ is represented by the component matrix $\mathbf{u}$ with components x, y, and z, the function A which produces the matrix representation of $\vec{u}\times$ from the component matrix $\mathbf{u}$ is

$$\mathsf{A}(\mathbf{u}) = \begin{bmatrix} 0 & -z & y \\ z & 0 & -x \\ -y & x & 0 \end{bmatrix}. \tag{2.36}$$

The inverse of this function can be applied to any skew-symmetric matrix, and so we can use A^{-1} to extract the components $\boldsymbol{\omega}$ of the angular velocity vector from the matrix representation of $\vec{\omega}\times$ in terms of M:

$$\boldsymbol{\omega} = \mathsf{A}^{-1}(D\mathbf{M}\ \mathbf{M}^{\mathrm{T}}), \tag{2.37}$$

where $\mathbf{M}$ and $D\mathbf{M}$ are the matrix representations of the functions M and DM, and where we have used the fact that for a matrix representation of a rotation the tranpose gives the inverse.

The components $\boldsymbol{\omega}'$ of the angular velocity vector on the principal axes are: $\boldsymbol{\omega}' = \mathbf{M}^{\mathrm{T}}\boldsymbol{\omega}$. So

$$\boldsymbol{\omega}' = \mathbf{M}^{\mathrm{T}}\mathsf{A}^{-1}(D\mathbf{M}\ \mathbf{M}^{\mathrm{T}}). \tag{2.38}$$

The relationship of the angular velocity vector to the path is a kinematic relationship; it is valid for any path. Thus we can abstract it to obtain the components of the angular velocity at a moment given the configuration and velocity at that moment.

Implementation of Angular Velocity Functions

The following procedure gives the components of the angular velocity as a function of time along the path

```
(define (((M-of-q->omega-of-t M-of-q) q) t)
  (define M-on-path (compose M-of-q q))
  (define (omega-cross t)
    (* ((D M-on-path) t)
       (m:transpose (M-on-path t))))
  (antisymmetric->column-matrix (omega-cross t)))
```

The procedure omega-cross produces the matrix representation of $\vec{\omega}\times$. The $\vec{\omega}\times$ matrix is antisymmetric and has components of the angular velocity vector $\vec{\omega}$. We can extract these components of the angular velocity vector with the procedure antisymmetric->column-matrix, which corresponds to the function A^{-1}. The body components of the angular velocity vector as a function of time along the path are

```
(define (((M-of-q->omega-body-of-t M-of-q) q) t)
  (* (m:transpose (M-of-q (q t)))
     (((M-of-q->omega-of-t M-of-q) q) t)))
```

We can get the procedures of local state that give the angular velocity components by abstracting these procedures along arbitrary paths that have given coordinates and velocities. The abstraction of a procedure of a path to a procedure of state is accomplished by Gamma-bar (see section 1.6.1):

```
(define (M->omega M-of-q)
  (Gamma-bar
    (M-of-q->omega-of-t M-of-q)))

(define (M->omega-body M-of-q)
  (Gamma-bar
    (M-of-q->omega-body-of-t M-of-q)))
```

These procedures give the angular velocities as a function of state. We will see them in action after we get some M-of-q's with which to work.

2.7 Euler Angles

To go further we must finally specify a set of generalized coordinates. We first do this using the traditional *Euler angles*. Later, we find other ways of describing the orientation of a rigid body.

We are using an intermediate representation of the orientation in terms of the function M of the generalized coordinates that gives the rotation that takes the body from some reference orientation and rotates it to the orientation specified by the generalized coordinates. Here we take the reference orientation so that principal-axis unit vectors $\hat{a}$, $\hat{b}$, $\hat{c}$ are coincident with the basis vectors $\hat{e}_i$ labeled here by $\hat{x}$, $\hat{y}$, $\hat{z}$.

We define the Euler angles in terms of simple rotations about the coordinate axes. Let $R_x(\psi)$ be a right-handed rotation about the $\hat{x}$ axis by the angle ψ, and let $R_z(\psi)$ be a right-handed rotation about the $\hat{z}$ axis by the angle ψ. The function M for Euler angles is written as a composition of three of these simple coordinate axis rotations:

$$\mathsf{M}(\theta, \varphi, \psi) = R_z(\varphi)R_x(\theta)R_z(\psi), \tag{2.39}$$

for the Euler angles θ, φ, ψ.

The Euler angles can specify any orientation of the body, but the orientation does not always correspond to a unique set of Euler angles. In particular, if $\theta = 0$ then the orientation is dependent only on the sum $\varphi + \psi$, so the orientation does not uniquely determine either φ or ψ.

Exercise 2.8: Euler Angles

It is not immediately obvious that all orientations can be represented in terms of the Euler angles. To show that Euler angles are adequate to represent all orientations solve for Euler angles that give an arbitrary rotation R. Keep in mind that some orientations do not correspond to a unique representation in terms of Euler angles.

Though the Euler angles allow us to specify all orientations and thus can be used as generalized coordinates, the definition of Euler angles is pretty arbitrary. In fact no reasoning has led us to them, and this is reflected in our presentation of them by just saying "here they are." Euler angles are well suited for some problems and are cumbersome for others.

There are other ways of defining similar sets of angles. For instance, we could also take our generalized coordinates to satisfy

$$\mathsf{M}'(\theta, \varphi, \psi) = R_x(\varphi)R_y(\theta)R_z(\psi). \tag{2.40}$$

Such alternatives to the Euler angles come in handy from time to time.

Each of the fundamental rotations can be represented as a matrix. The rotation matrix representing a right-handed rotation about the $\hat{z}$ axis by the angle ψ is

$$\mathbf{R}_z(\psi) = \begin{bmatrix} \cos\psi & -\sin\psi & 0 \\ \sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{2.41}$$

and a right-handed rotation about the x axis by the angle ψ is represented by the matrix

$$\mathbf{R}_x(\psi) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\psi & -\sin\psi \\ 0 & \sin\psi & \cos\psi \end{bmatrix}. \tag{2.42}$$

The matrix that represents the rotation that carries the body from its reference orientation to the actual orientation is

$$\mathbf{R}_z(\varphi)\mathbf{R}_x(\theta)\mathbf{R}_z(\psi). \tag{2.43}$$

The rotation matrices and their product can be constructed by simple programs:

```
(define (rotate-z angle)
  (matrix-by-rows
    (list (cos angle) (- (sin angle))              0)
    (list (sin angle)     (cos angle)              0)
    (list           0               0              1)))

(define (rotate-x angle)
  (matrix-by-rows
    (list           1               0              0)
    (list           0     (cos angle) (- (sin angle)))
    (list           0     (sin angle)     (cos angle))))

(define (Euler->M angles)
  (let ((theta (ref angles 0))
        (phi (ref angles 1))
        (psi (ref angles 2)))
    (* (rotate-z phi)
       (rotate-x theta)
       (rotate-z psi))))
```

Now that we have a procedure that implements a sample M, we can find the components of the angular velocity vector and the body components of the angular velocity vector using the procedures `M-of-q->omega-of-t` and `M-of-q->omega-body-of-t` from section 2.6. For example,

```
(show-expression
 (((M-of-q->omega-body-of-t Euler->M)
   (coordinate-tuple (literal-function 'theta)
                     (literal-function 'phi)
                     (literal-function 'psi)))
  't))
```

$$\begin{bmatrix} D\varphi(t)\sin(\theta(t))\sin(\psi(t)) + \cos(\psi(t))\,D\theta(t) \\ D\varphi(t)\sin(\theta(t))\cos(\psi(t)) - \sin(\psi(t))\,D\theta(t) \\ \cos(\theta(t))\,D\varphi(t) + D\psi(t) \end{bmatrix}$$

To construct the kinetic energy we need the procedure of state that gives the body components of the angular velocity vector:

```
(show-expression
 ((M->omega-body Euler->M)
  (->local 't
           (coordinate-tuple 'theta 'phi 'psi)
           (velocity-tuple 'thetadot 'phidot 'psidot))))
```

$$\begin{bmatrix} \dot\varphi\sin(\psi)\sin(\theta) + \dot\theta\cos(\psi) \\ \dot\varphi\sin(\theta)\cos(\psi) - \dot\theta\sin(\psi) \\ \dot\varphi\cos(\theta) + \dot\psi \end{bmatrix}$$

We capture this result as a procedure:

```
(define (Euler-state->omega-body local)
  (let ((t (time local))
        (q (coordinate local))
        (qdot (velocity local)))
    (let ((theta (ref q 0))
          (psi (ref q 2))
          (thetadot (ref qdot 0))
          (phidot (ref qdot 1))
          (psidot (ref qdot 2)))
      (let ((omega-a (+ (* thetadot (cos psi))
                        (* phidot (sin theta) (sin psi))))
            (omega-b (+ (* -1 thetadot (sin psi))
                        (* phidot (sin theta) (cos psi))))
            (omega-c (+ (* phidot (cos theta)) psidot)))
        (column-matrix omega-a omega-b omega-c)))))
```

The kinetic energy can be written:

```
(define ((T-rigid-body A B C) local)
  (let ((omega-body (Euler-state->omega-body local)))
    (* 1/2
       (+ (* A (square (ref omega-body 0)))
          (* B (square (ref omega-body 1)))
          (* C (square (ref omega-body 2)))))))
```

2.8 Vector Angular Momentum

The vector angular momentum of a particle is the cross product of the position and the linear momentum. For a rigid body the vector angular momentum is the sum of the vector angular momentum of each of the constituents. Here we find an expression for the vector angular momentum of a rigid body in terms of the inertia tensor and the angular velocity vector.

The vector angular momentum of a rigid body is:

$$\sum_\alpha \vec{x}_\alpha \times (m_\alpha \dot{\vec{x}}_\alpha), \tag{2.44}$$

where $\vec{x}_\alpha$, $\dot{\vec{x}}_\alpha$, and m_α are the positions, velocities, and masses of the constituent particles. It turns out that the vector angular momentum decomposes into the sum of the angular momentum of the center of mass and the rotational angular momentum about the center of mass, just as the kinetic energy separates into the kinetic energy of the center of mass and the kinetic energy of rotation. As in the kinetic energy demonstration, decompose the position into the vector to the center of mass $\vec{X}$ and the vectors from the center of mass to the constituent mass elements $\vec{\xi}_\alpha$:

$$\vec{x}_\alpha = \vec{X} + \vec{\xi}_\alpha, \tag{2.45}$$

with velocities

$$\dot{\vec{x}}_\alpha = \dot{\vec{X}} + \dot{\vec{\xi}}_\alpha. \tag{2.46}$$

Substituting, the angular momentum is

$$\sum_\alpha m_\alpha (\vec{X} + \vec{\xi}_\alpha) \times (\dot{\vec{X}} + \dot{\vec{\xi}}_\alpha). \tag{2.47}$$

Multiplying out the product, and using the fact that $\vec{X}$ is the center of mass, and $M = \sum_\alpha m_\alpha$ is the total mass of the body, the angular momentum is

$$\vec{X} \times (M\dot{\vec{X}}) + \sum_\alpha \vec{\xi}_\alpha \times (m_\alpha \dot{\vec{\xi}}_\alpha). \tag{2.48}$$

The angular momentum of the center of mass is

$$\vec{X} \times (M\dot{\vec{X}}), \tag{2.49}$$

and the rotational angular momentum is

$$\sum_\alpha \vec{\xi}_\alpha \times (m_\alpha \dot{\vec{\xi}}_\alpha). \tag{2.50}$$

We can also reexpress the rotational angular momentum in terms of the angular velocity vector and the inertia tensor, as we did for the kinetic energy. Using $\dot{\vec{\xi}}_\alpha = \vec{\omega} \times \vec{\xi}_\alpha$. The rotational angular momentum is

$$\vec{L} = \sum_\alpha m_\alpha \vec{\xi}_\alpha \times (\vec{\omega} \times \vec{\xi}_\alpha). \tag{2.51}$$

In terms of components with respect to the basis $\hat{e}_i$, this is

$$L_j = \sum_k I_{jk} \omega^k, \tag{2.52}$$

where I_{jk} are the components of the inertia tensor (2.14). The angular momentum and the kinetic energy are expressed in terms of the same inertia tensor.

With respect to the principal axis basis, the angular momentum components have a particularly simple form:

$$L_a = A\omega^a \tag{2.53}$$
$$L_b = B\omega^b \tag{2.54}$$
$$L_c = C\omega^c. \tag{2.55}$$

Exercise 2.9:

Verify that the expression (2.52) for the components of the rotational angular momentum (2.51) in terms of the inertia tensor is correct.

We can define procedures to calculate the components of the angular momentum on the principal axes:

```
(define ((Euler-state->L-body A B C) local)
  (let ((omega-body (Euler-state->omega-body local)))
    (column-matrix (* A (ref omega-body 0))
                   (* B (ref omega-body 1))
                   (* C (ref omega-body 2)))))
```

We then transform the components of the angular momentum on the principal axes to the components on the fixed basis $\hat{e}_i$:

```
(define ((Euler-state->L-space A B C) local)
  (let ((angles (coordinate local)))
    (* (Euler->M angles)
       ((Euler-state->L-body A B C) local))))
```

These procedures are local state functions, like Lagrangians.

2.9 Motion of a Free Rigid Body

The kinetic energy, expressed in terms of a suitable set of generalized coordinates, is a Lagrangian for a free rigid body. In Section 2.1 we found that the kinetic energy of a rigid body can be written as the sum of the rotational kinetic energy and the translational kinetic energy. By choosing one set of coordinates to specify the position and another set to specify the orientation the Lagrangian becomes a sum of a translational Lagrangian and a rotational Lagrangian. The Lagrange equations for translational motion are not coupled to the Lagrange equations for the rotational motion. For a free rigid body the translational motion is just that of a free particle: uniform motion. Here we concentrate on the rotational motion of the free rigid body. We can adopt the Euler angles as the coordinates that specify the orientation; the rotational kinetic energy was expressed in terms of Euler angles in the previous section.

Conserved Quantities

The Lagrangian for a free rigid body has no explicit time dependence, so we can deduce that the energy, which is just the kinetic energy, is conserved by the motion.

The Lagrangian does not depend on the Euler angle φ, so we can deduce that the momentum conjugate to this coordinate is conserved. An explicit expression for the momentum conjugate to φ is:

```
(define an-Euler-state
  (->local 't
           (coordinate-tuple 'theta 'phi 'psi)
           (velocity-tuple 'thetadot 'phidot 'psidot)))

(show-expression
 (ref (((partial 2) (T-rigid-body 'A 'B 'C)) an-Euler-state)
      1))
```

$$\begin{aligned}
&A\dot{\varphi}\left(\sin\left(\theta\right)\right)^2\left(\sin\left(\psi\right)\right)^2 + A\dot{\theta}\cos\left(\psi\right)\sin\left(\theta\right)\sin\left(\psi\right)\\
&\quad + B\dot{\varphi}\left(\cos\left(\psi\right)\right)^2\left(\sin\left(\theta\right)\right)^2 - B\dot{\theta}\cos\left(\psi\right)\sin\left(\theta\right)\sin\left(\psi\right)\\
&\quad + C\dot{\varphi}\left(\cos\left(\theta\right)\right)^2 + C\dot{\psi}\cos\left(\theta\right)
\end{aligned}$$

We know that this complicated quantity is conserved by the motion of the rigid body because of the symmetries of the Lagrangian.

If there are no external torques, then we expect that the vector angular momentum will be conserved. We can verify this using the Lagrangian formulation of the problem. First, we note that L_z is the same as p_φ. We can check this by direct calculation:

```
(print-expression
 (- (ref ((Euler-state->L-space 'A 'B 'C) an-Euler-state)
         2)
    (ref (((partial 2) (T-rigid-body 'A 'B 'C)) an-Euler-state)
         1)))
;Value: 0
```

We know that p_φ is conserved because the Lagrangian for the free rigid body did not mention φ, so now we know that L_z is conserved. Since the orientation of the coordinate axes is arbitrary, we know that if any rectangular component is conserved then all of them are. So the vector angular momentum is conserved for the free rigid body.

Of course, we could have seen this with the help of Noether's theorem (see section 1.9.4). There are a continuous family of rotations that can transform any orientation into any other orientation. The orientation of the coordinate axes we used to define the Euler angles is arbitrary, and the kinetic energy (the Lagrangian) is the same for any choice of coordinate system. Thus the situation meets the requirements of Noether's theorem, which tells us that there is a conserved quantity. In particular, the family of rotations around each coordinate axis gives us conservation of the angular momentum component on that axis. We construct the vector angular momentum by combining these contributions.

Exercise 2.10: Vector Angular Momentum

Fill in the details of the argument that Noether's theorem implies that vector angular momentum is conserved by the motion of the free rigid body.

2.9.1 Computing the motion of free rigid bodies

Lagrange's equations for the motion of a free rigid body in terms of Euler angles are quite disgusting, so we will not show them here. However, we will use the Lagrange equations to explore the motion of the free rigid body.

Before doing this it is worth noting that the equations of motion in Euler angles are singular for some configurations, because for these configurations the Euler angles are not uniquely defined. If we set $\theta = 0$ then an orientation does not correspond to a unique value of φ and ψ; only their sum determines the orientation.

The singularity arises in the explicit Lagrange equations when we attempt to solve for the second derivative of the generalized coordinates in terms of the generalized coordinates and the generalized velocities (see section 1.8). The isolation of the second derivative requires multiplying by the inverse of $\partial_2\partial_2 L$. The determinant of this quantity becomes zero when the Euler angle θ is zero.

```
(show-expression
 (determinant
  (((compose (partial 2) (partial 2))
    (T-rigid-body 'A 'B 'C))
   an-Euler-state)))
```

$$\boxed{ABC\,(\sin(\theta))^2}$$

So when θ is zero, we cannot solve for the second derivatives. When θ is small, the Euler angles can move very rapidly, and thus may be difficult to compute reliably. Of course, the motion of the rigid body is perfectly well behaved for any orientation. This is a problem of the representation of that motion in Euler angles; it is a "coordinate singularity."

One solution to this problem is to use another set of Euler-like coordinates for which Lagrange's equations have singularities for different orientations, such as those defined in equation (2.40). So as the calculation proceeds, if we come close to a singularity in one set of coordinates we can switch and use the other set for a while until they encounter a singularity. This solves the problem, but it is cumbersome. For the moment we will ignore this problem and compute some trajectories, being careful to limit our attention to trajectories that avoid the singularities.

We will compute some trajectories by numerical integration and check our integration process by seeing how well energy and angular momentum are conserved. Then, we will investigate the evolution of the components of angular momentum on the principal axis basis. We will discover that we can learn quite a bit about the qualitative behavior of rigid bodies by combining the information we get from the energy and angular momentum.

To develop a trajectory from initial conditions we integrate the Lagrange equations, as we did in Chapter 1: we take the Lagrangian for the free rigid body that we have developed, compile a system derivative, and make and use appropriate integrators and plotters.

The system derivative is obtained from the Lagrangian, and compiled:

```
(define (rigid-sysder A B C)
  (Lagrangian->state-derivative (T-rigid-body A B C)))

(define rigid-sysder-compiled
  (compile-parametric 7 rigid-sysder))
```

The following program integrates the equations of motion for a free rigid body, given initial conditions. It plots the relative error in the three angular momentum components and in the energy:

```
(define (do-it A B C istate0 final-t dt tol)
  (let ((dstate (rigid-sysder-compiled A B C))
        (local0 (istate->local istate0)))
    (let ((L0 ((Euler-state->L-space A B C) local0))
          (E0 ((T-rigid-body A B C) local0)))
      (let loop ((istate istate0))
        (if (< (istate->t istate) final-t)
            (let ((ns (ode-advancer dstate istate dt tol)))
              (let ((local (istate->local ns)))
                (let ((L ((Euler-state->L-space A B C) local))
                      (E ((T-rigid-body A B C) local)))
                  (plot-errors (time local) L0 E0 L E)))
              (loop ns)))))))

(define (plot-errors t L0 E0 L E)
  (let ((Lx0 (ref L0 0)) (Ly0 (ref L0 1)) (Lz0 (ref L0 2))
        (Lx (ref L 0)) (Ly (ref L 1)) (Lz (ref L 2)))
    (plot-point window t (relative-error Lx Lx0))
    (plot-point window t (relative-error Ly Ly0))
    (plot-point window t (relative-error Lz Lz0))
    (plot-point window t (relative-error E E0))))

(define (relative-error value reference-value)
  (if (zero? reference-value)
      (error "Zero reference value -- RELATIVE-ERROR")
      (/ (- value reference-value) reference-value)))
```

To build our plot we make a window with a scale appropriate to the expected relative errors and we run our program:

```
(define window (frame 0. 100. -1.e-12 1.e-12))
```

```
(do-it 1. (sqrt 2.) 2.          ; principal moments
       (->istate
         0.0                    ; initial conditions
         (coordinate-tuple 1. 0. 0.)
         (velocity-tuple 0.1 0.1 0.1))
       100.0                    ; final time
       0.1                      ; step between plotted points
       1.0e-12)                 ; max local truncation error
```

The plot that is developed of the relative errors in the components of the angular momenta and the energy (see Figure 2.2) shows that we have been successful in controlling the error in the conserved quantities. This should give us some confidence in the trajectory that is evolved.

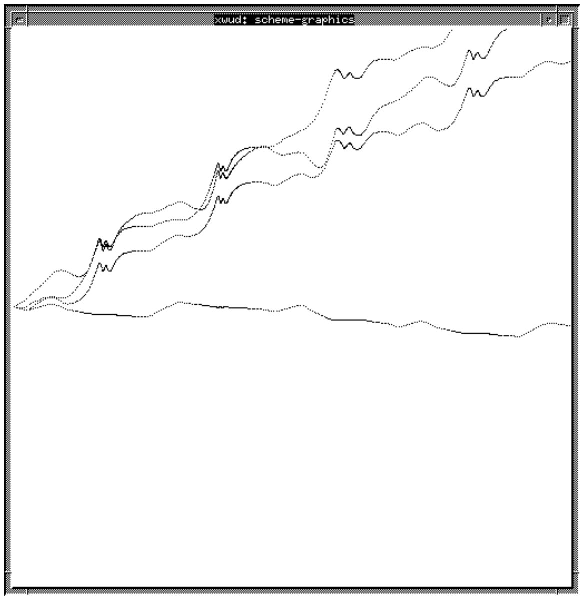

Figure 2.2 The relative error in energy and in the three spatial components of the angular momentum. The ordinate scale spans $\pm 10^{-12}$, and the abscissa is time from 0 to 100. It is interesting to note that the energy error is one of the three rising curves.

2.9.2 Qualitative Features of Free Rigid Body Motion

The evolution of the components of the angular momentum on the principal axes has a remarkable property. For almost every initial condition the body components of the angular momentum periodically trace a simple closed curve.

We can see this by investigating a number of trajectories, and plotting the components of angular momentum of the body on the principal axes (see figure 2.3). We find a non-intersecting set of one-dimensional simple-closed curves. To make this figure a number of trajectories of equal energy were computed. The three dimensional space of body components is projected onto a two-dimensional plane for display. The trajectories appear to cross only because they are projected.

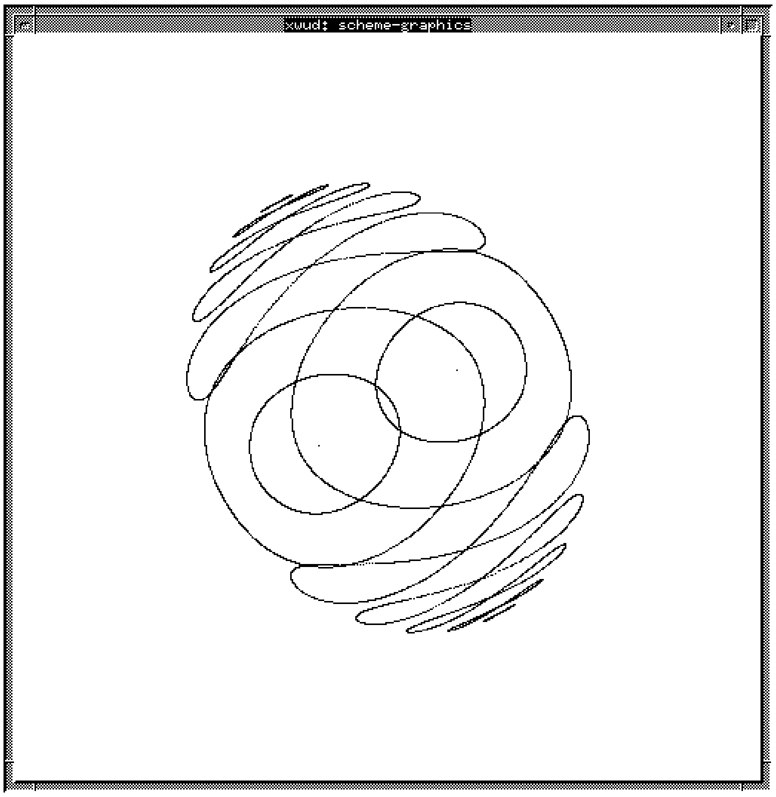

Figure 2.3 Trajectories of the components of the angular momentum vector on the principal axes, projected onto a plane. Each closed curve is a different trajectory. All the trajectories shown here have the same energy.

What is going on? The state space for a free rigid body is six dimensional: the three Euler angles and their time derivatives.

We know four constants of the motion — the three spatial components of the angular momentum, L_x, L_y, and L_z, and the energy, E. Thus, the motion is restricted to a two-dimensional region of the state space.[9] Our experiment shows that the components of the angular momentum trace one-dimensional closed curves in the angular-momentum subspace, so there is something more going on here.

The total angular momentum is conserved if all of the components are, so we also have the constant

$$L^2 = L_x^2 + L_y^2 + L_z^2. \tag{2.56}$$

The spatial components of the angular momentum do not change, but of course the projections of the angular momentum onto the principal axes do change because the axes move as the body moves. However, the magnitude of the angular momentum vector is the same whether it is computed from components on the fixed basis or components on the principal axis basis. So, the combination

$$L^2 = L_a^2 + L_b^2 + L_c^2, \tag{2.57}$$

is conserved.

Using the expressions (2.53 - 2.55) for the angular momentum in terms of the components of the angular velocity vector on the principal axes, the kinetic energy (2.30) can be rewritten in terms of the angular momentum components on the principal axes

$$E = \frac{1}{2}\left(\frac{L_a^2}{A} + \frac{L_b^2}{B} + \frac{L_c^2}{C}\right). \tag{2.58}$$

The two integrals (2.57 and 2.58) provide constraints on how the components of the angular momentum vector on the principal axes can change. We recognize the angular momentum integral (2.57) as the equation of a sphere, and the kinetic energy integral (2.58) as the equation for a triaxial ellipsoid. Both integrals are conserved so the components of the angular momentum are constrained to move on the intersection of these two surfaces,

[9] We expect that for each constant of the motion we reduce by one the dimension of the region of the state space explored by a trajectory. This is because a constant of the motion can be used to locally solve for one of the state variables in terms of the others.

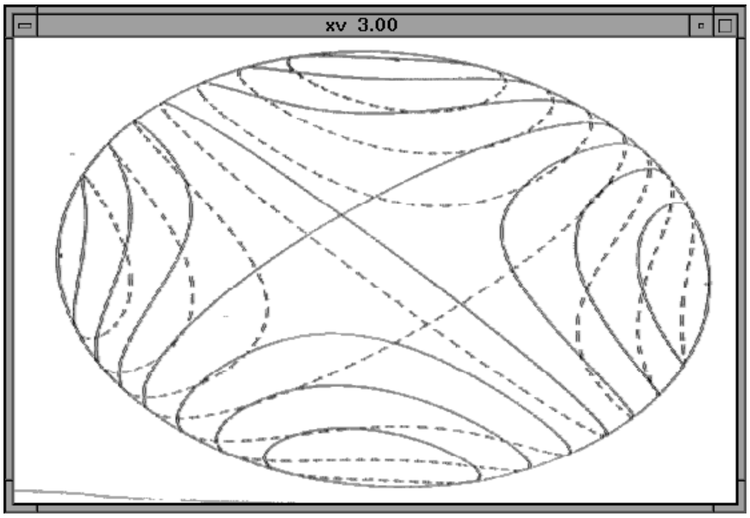

Figure 2.4 Trajectories on the energy ellipsoid in terms of the components of the angular momentum on the principal axes.

the energy ellipsoid and the angular momentum sphere (see Figure 2.4). The intersection of an ellipsoid and a sphere with the same center is generically two closed curves, so an orbit is confined to one of these curves. This sheds light on the puzzle at the beginning of this section.

Because of our ordering $A \leq B \leq C$, the longest axis of this triaxial ellipsoid coincides with the $\hat{c}$ direction, when all the angular momentum is along the axis of largest principal moment of inertia, and the shortest axis of the energy ellipsoid coincides with the $\hat{a}$ axis, when all the angular momentum is along the smallest moment of inertia. Without actually solving the Lagrange equations, we have found strong constraints on the evolution of the components of the angular momentum on the principal axes.

To determine how the system evolves along these intersection curves we have to use the equations of motion. We observe that the evolution of the components of the angular momentum on the principal axes depends only on the components of the angular momentum on the principal axes, even though the values of these components are not enough to completely specify the dynamical state. Apparently the dynamics of these components is self contained, and we will see that it can be described in terms of a set of differential equations whose only dynamical variables are the components of the angular momentum on the principal axes (see section 2.12).

We note that there are two axes for which the intersection curves shrink to a point if we hold the energy constant and vary the magnitude of the angular momentum. If the angular momentum starts at these points, the integrals constrain the angular momentum to stay there. These points are *equilibrium* points for the body components of the angular momentum. However, these points are not equilibrium points for the system as a whole. At these points the body is still rotating even though the body components of the angular momentum are not changing. This kind of equilibrium is called a *relative equilibrium*. We can also see that if the angular momentum is initially slightly displaced from one of these relative equilibria then the angular momentum is constrained to stay near it on one of the intersection curves. The angular momentum vector is fixed in space, so the principal axis of the equilibrium point of the body rotates stably about the angular momentum vector.

At the principal axis with intermediate moment of inertia, the $\hat{b}$ axis, the intersection curves cross. As we observed, the dynamics of the components of the angular momentum on the principal axes form a self-contained dynamical system. Trajectories of a dynamical system cannot cross,[10] so the most that can happen is that if the equations of motion carry the system along the intersection curve then the system can only asymptotically approach the crossing point. So without solving any equations we can deduce that the point of crossing is another relative equilibrium. If the angular momentum is initially aligned with the intermediate axis, then it stays aligned. If the system is slightly displaced from the intermediate axis, then the evolution along the intersection curve will take the system far from the relative equilibrium. So rotation about the axis of intermediate moment of inertia is unstable — initial displacements of the angular momentum, however small initially, become large. Again, the angular momentum vector is fixed in space, but now the principal axis with the intermediate principal moment does not stay close to the angular momentum, so the body executes a complicated tumbling motion.

This gives some insight into the mystery of the thrown book mentioned at the beginning of the chapter. If one throws a book

[10]Systems of ODEs that satisfy a Lipschitz condition have unique solutions.

so that it is initially rotating about either the axis with the largest or the smallest moment of inertia (the smallest and largest physical axes, respectively), the book rotates regularly about that axis. However, if the book is thrown so that it is initially rotating about the axis of intermediate moment of inertia (the intermediate physical axis), then the book tumbles, however carefully the book is thrown. You can try it with this book (but put a rubber band around it first).

Before moving on, we can make some further physical deductions. Suppose a freely rotating body is subject to some sort of internal friction that dissipates energy, but conserves the angular momentum. For example, real bodies flex as they spin. If the spin axis moves with respect to the body then the flexing changes with time, and this changing distortion converts kinetic energy of rotation into heat. Internal processes do not change the total angular momentum of the system. If we hold the magnitude of the angular momentum fixed but gradually decrease the energy then the curve of intersection on which the system moves gradually deforms. For a given angular momentum there is a lower limit on the energy; the energy cannot be so low that there are no intersections. For this lowest energy the intersection of the angular momentum sphere and the energy ellipsoid is a pair of points on the axis of maximum moment of inertia. With energy dissipation, a freely rotating physical body eventually ends up with the lowest energy consistent with the given angular momentum, which is rotation about the principal axis with the largest moment of inertia (typically the shortest physical axis).

Thus, we expect that given enough time all freely rotating physical bodies will end up rotating about the axis of largest moment of inertia. You can demonstrate this to your satisfaction by twirling a small bottle containing some viscous fluid, such as correction fluid. What you will find is that, whatever spin you try to put on the bottle, it will reorient itself so that the axis of the largest moment of inertia is aligned with the spin axis. Remarkably, this is very nearly true of almost every body in the solar system for which there is enough information to decide. The deviations from principal axis rotation for the Earth are tiny, the angle between the angular momentum vector and the $\hat{c}$ axis for the Earth is less than one arc-second.[11] In fact, the evidence is that all of the planets, the Moon and all of the other natural satellites, and almost all of the asteroids rotate very nearly about the largest moment of inertia. We have deduced that this is to be expected using an elementary argument. There are exceptions. Comets typically do not rotate about the largest moment. As they are heated by the sun, material spews out from localized jets, and the back reaction from these jets changes the rotation state. Among the natural satellites, the only known exception is Saturn's satellite Hyperion, which is tumbling chaotically. Hyperion is especially out-of-round and subject to strong gravitational torques from Saturn.

2.10 Axisymmetric Tops

We have all played with a top at one time or another. For the purposes of analysis we will consider an idealized top that does not wander around. Thus, an ideal top is a rotating rigid body, one point of which is fixed in space. Furthermore, the center of mass of the top is not at the fixed point, which is the center of rotation, and there is a uniform gravitational acceleration.

For our top we can take the Lagrangian to be the difference of the kinetic energy and the potential energy. We already know how to write the kinetic energy — what is new here is that we must express the potential energy in terms of the configuration. In the case of a body in a uniform gravitational field this is easy. The potential energy is sum of "mgh" for all the constituent particles:

$$\sum_\alpha m_\alpha g h_\alpha, \tag{2.59}$$

where g is the gravitational acceleration, $h_\alpha = \vec{x}_\alpha \cdot \hat{z}$, and where the unit vector $\hat{z}$ indicates which way is up. Rewriting the vector to the constituents in terms of the vector $\vec{X}$ to the center of mass, the potential energy is:

$$\sum_\alpha m_\alpha g \left(\vec{X} + \vec{\xi}_\alpha\right) \cdot \hat{z}$$

[11] The deviation of the angular momentum from the principal axis may be due to a number of effects: earthquakes, atmospheric tides, ...

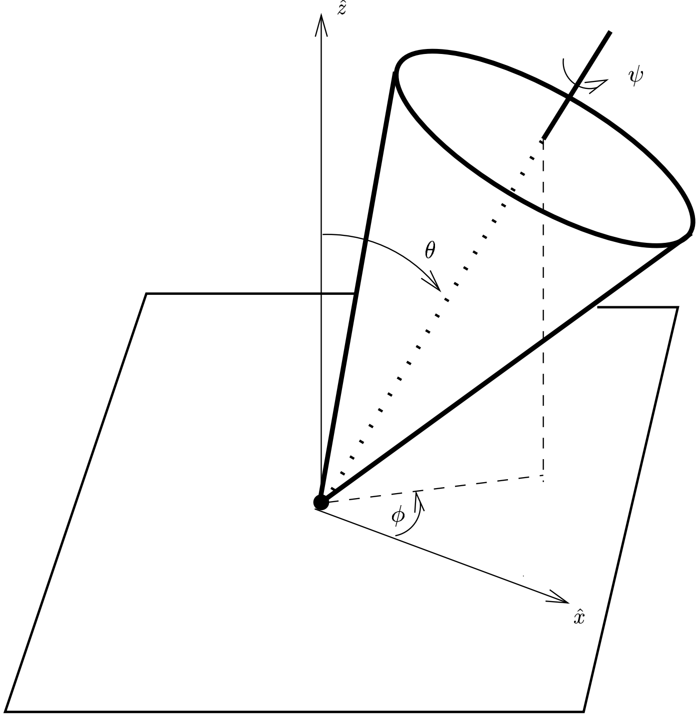

Figure 2.5 An axisymmetric top is a symmetrical rigid body in a uniform gravitational field with one point of the body fixed in space. The Euler angles used to specify the configuration are indicated.

$$
\begin{aligned}
&= gM\vec{X} \cdot \hat{z} + g\left(\sum_\alpha m_\alpha \vec{\xi}_\alpha\right) \cdot \hat{z} \\
&= gM\vec{X} \cdot \hat{z}, \qquad (2.60)
\end{aligned}
$$

where the last sum is zero because the center of mass is the origin of $\vec{\xi}_\alpha$. So the potential energy of a body in a gravitational field with uniform acceleration is very simple: it is just Mgh, where M is the total mass, and $h = \vec{X} \cdot \hat{z}$ is the height of the center of mass.

Here we consider an axisymmetric top (see figure 2.5). Such a top has an axis of symmetry of the mass distribution, so the center of mass is on the symmetry axis, and the fixed point is also on the axis of symmetry.

In order to write the Lagrangian we need to choose a set of generalized coordinates. If we choose them well we can take advantage of the symmetries of the problem. If the Lagrangian does not depend on a particular coordinate the conjugate momentum is conserved, and the complexity of the system is reduced.

The axisymmetric top has two apparent symmetries. The fact that the mass distribution is axisymmetric implies that neither the kinetic nor potential energy is sensitive to the orientation of the top about that symmetry axis. Additionally, the kinetic and potential energy are insensitive to a rotation of the physical system about the vertical axis, because the gravitational field is uniform.

We can take advantage of these symmetries by choosing appropriate coordinates, and we already have a coordinate system that does the job — the Euler angles.[12] We choose the reference orientation so that the symmetry axis is vertical. The first Euler angle ψ expresses a rotation about the symmetry axis. The next Euler angle θ is the tilt of the symmetry axis of the top from the vertical. The third Euler angle φ expresses a rotation of the top about the z axis. The symmetries of the problem imply that the first and third Euler angles do not appear in the Lagrangian. As a consequence the momenta conjugate to these angles are conserved quantities. Let's work out the details.

First, we work out the Lagrangian explicitly. The general form of the kinetic energy has been worked out, but here there is one twist. The top is constrained so that it pivots about a fixed point that is not at the center of mass. So the moments of inertia that enter the kinetic energy are the moments of inertia of the top with respect to the pivot point, not about the center of mass. If we know the moments of inertia about the center of mass we can write the moments of inertia about the pivot in terms of them (see Exercise 2.2). So let's assume the principal moments of inertia of the top about the pivot are A, B, and C, and $A = B$ because of the symmetry.[13] We can use the computer to help us figure out the Lagrangian for this special case:

---

[12]That the axisymmetric top can be solved in Euler angles is, no doubt, the reason for the traditional choice of the definition of the Euler angles. For other problems, the Euler angles may offer no particular advantage.

[13]Here, we do not require that C be larger than $A = B$, because they are not measured with respect to the center of mass.

```
(show-expression
 ((T-rigid-body 'A 'A 'C)
   (->local 't
            (coordinate-tuple 'theta 'phi 'psi)
            (velocity-tuple 'thetadot 'phidot 'psidot))))
```

$$\boxed{\frac{1}{2}(\sin(\theta))^2 A\dot{\varphi}^2 + \cos(\theta)\left(\frac{1}{2}\cos(\theta) C\dot{\varphi}^2 + C\dot{\varphi}\dot{\psi}\right) + \frac{1}{2}A\dot{\theta}^2 + \frac{1}{2}C\dot{\psi}^2}$$

We can rearrange this a bit to get

$$T(t;\theta,\varphi,\psi;\dot{\theta},\dot{\varphi},\dot{\psi}) \\ = \tfrac{1}{2}A\left(\dot{\theta}^2 + \dot{\varphi}^2\sin^2\theta\right) + \tfrac{1}{2}C\left(\dot{\psi} + \dot{\varphi}\cos\theta\right)^2. \tag{2.61}$$

In terms of Euler angles, the potential energy is

$$V(t;\theta,\varphi,\psi;\dot{\theta},\dot{\varphi},\dot{\psi}) = MgR\cos\theta, \tag{2.62}$$

where R is the distance of the center of mass from the pivot. The Lagrangian is $L = T - V$. We see that the Lagrangian is indeed independent of ψ and φ, as expected.

There is no particular reason to look at the Lagrange equations. We can assign that job to the computer when needed. However, we have already seen that it may be useful to examine the conserved quantities associated with the symmetries.

The energy is conserved, because the Lagrangian has no explicit time dependence. Also, the energy is the sum of the kinetic and potential energy $E = T + V$, because the kinetic energy is a homogeneous quadratic form in the generalized velocities. The energy is

$$E = \tfrac{1}{2}A\left(\dot{\theta}^2 + \dot{\varphi}^2\sin^2\theta\right) + \tfrac{1}{2}C\left(\dot{\psi} + \dot{\varphi}\cos\theta\right)^2 + MgR\cos\theta. \tag{2.63}$$

Two of the generalized coordinates do not appear in the Lagrangian, so there are two conserved momenta. The momentum conjugate to φ is

$$p_\varphi = \left(A(\sin\theta)^2 + C(\cos\theta)^2\right)\dot{\varphi} + C\dot{\psi}\cos\theta. \tag{2.64}$$

The momentum conjugate to ψ is

$$p_\psi = C(\dot{\psi} + \dot{\varphi}\cos\theta). \tag{2.65}$$

The state of the system at a moment is specified by the tuple $(t; \theta, \varphi, \psi; \dot{\theta}, \dot{\varphi}, \dot{\psi})$. The two coordinates φ and ψ that do not appear in the Lagrangian do not appear in the Lagrange equations or the conserved momenta. So the evolution of the remaining four state variables, θ, $\dot{\theta}$, $\dot{\varphi}$, and $\dot{\psi}$, depends only on those remaining state variables. This subsystem for the top has a four dimensional state space. The variables that did not appear in the Lagrangian can be determined by integrating the derivatives of these variables, which are determined separately by solving the independent subsystem.

The evolution of the top is described by a four-dimensional subsystem and two auxilliary quadratures.[14] This subdivision is a consequence of choosing generalized coordinates that incorporate the symmetries. However, the choice of generalized coordinates that incorporate the symmetries also gives conserved momenta. We can make use of these momenta to further simplify the formulation of the problem. Each integral can be used to locally eliminate one dimension of the subsystem. In this case the subsystem has four dimensions and there are three integrals, so the system can be completely reduced to quadratures. For the top, this can be done analytically, but we think it is a waste of time to do it. Rather, we are interested in extracting interesting features of the motion. We concentrate on the energy integral and use the two conserved momenta to eliminate $\dot{\varphi}$ and $\dot{\psi}$. After a bit of algebra we find:

$$E = \frac{1}{2}A\dot{\theta}^2 + \frac{(p_\varphi - p_\psi \cos\theta)^2}{2A(\sin\theta)^2} + \frac{p_\psi^2}{2C} + MgR\cos\theta. \tag{2.66}$$

Along a path θ, where $D\theta(t)$ is substituted for $\dot{\theta}$, this is an ordinary differential equation for θ. This differential equation involves various constants, some of which are set by the initial conditions of the other state variables. The solution of the differential equation for θ involves no more than ordinary integrals. So the top is essentially solved. We could continue this argument to obtain the qualitative behavior of θ: Using the energy (2.66), we can plot the trajectories in the plane of $\dot{\theta}$ versus θ, and see that the motion of θ is simply periodic. However we will defer continuing along

[14] Traditionally, evaluating a definite integral is known as performing a quadrature.

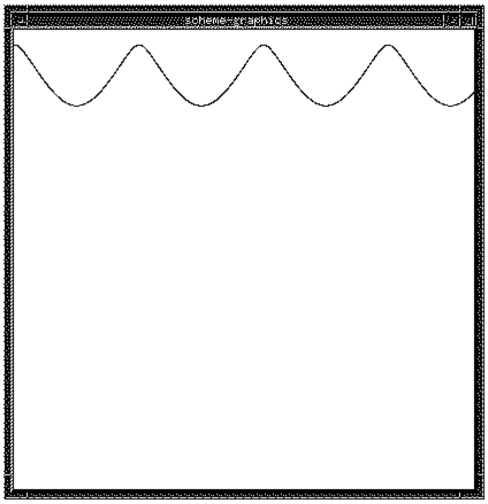

Figure 2.6 The tilt angle $\pi - \theta$ of the top versus time. The scale on the ordinate is 0 to π. The time interval on the abscissa is 2 seconds. The tilt of the top varies periodically.

this path until Chapter 3, when we have developed more tools for analysis.

Let's get real. Let's make a top out of a disk of aluminum material with a steel rod through the center to make the pivot. Measuring the top very carefully we find that the moment of inertia of the top about the symmetry axis is about 6.60×10^{-5}kg m^2, and the moment of inertia about the pivot point is about 3.28×10^{-4}kg m^2. The combination gMR is about 0.0456 kg m^{2}sec^{-2}. We spin the top up with an initial angular velocity of $\dot{\psi} = 140$radians/second (about 1337 rpm). The top initially has $\dot{\theta} = \varphi = \psi = 0$ and is initially tilted with $\theta = 0.1$radians. We then kick it so that $\dot{\varphi} = -15$radians/second. The figures (2.6 - 2.9) display aspects of the evolution of the top for 2 seconds. The tilt of the top (measured by θ) varies in a periodic manner. The orientation about the vertical is measured by φ: we see that the top also precesses, and the rate of precession varies with θ. We also see that as the top bobs up and down the rate of rotation of the top oscillates — the top spins faster when it is more vertical. The plot of tilt versus the precession angle shows that in this case the top executes a looping motion. If we do not kick it, but just let it drop then

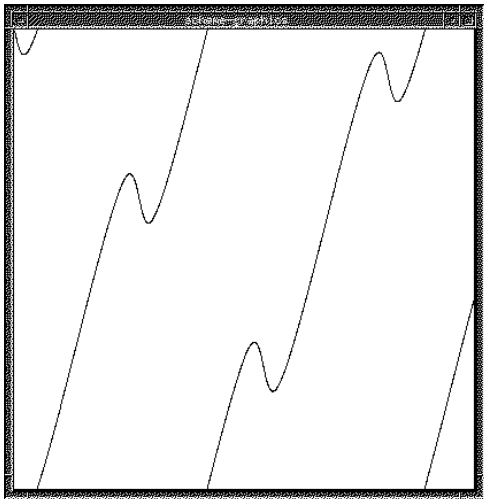

Figure 2.7 The precession angle φ of the top versus time. The scale on the ordinate is 0 to 2π radians. The time interval on the abscissa is 2 seconds. The top precesses nonuniformly — the rate of precession varies as the tilt varies.

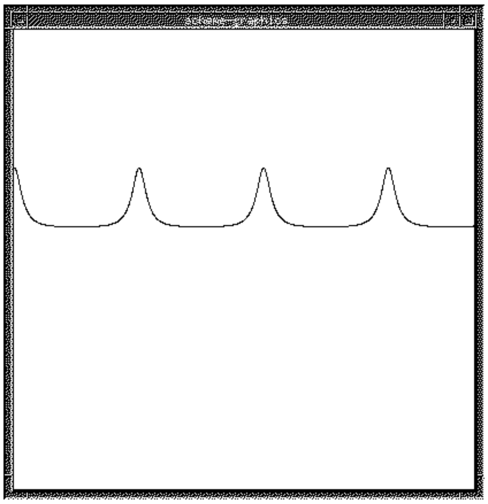

Figure 2.8 The rate of rotation $\dot{\psi}$ of the top versus time. The scale on the ordinate is 0 to 200 radians/second. The time interval on the abscissa is 2 seconds. The rate of rotation of the top changes periodically, as the tilt of the top varies.

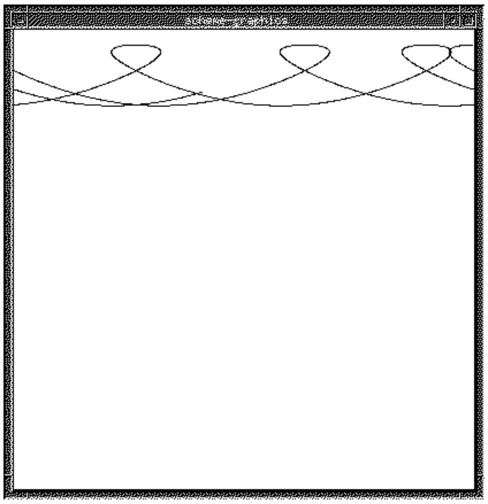

Figure 2.9 An idea of the actual motion of the top is obtained by plotting the tilt angle $\pi - \theta$ versus the precession angle φ. This is a "latitude-longitude" map showing the path of the center of mass of the top. We see that though the top has a net precession it executes a looping motion as it precesses.

the loop disappears leaving just a cusp. If we kick it in the other direction, then there is no cusp or any looping motion.

Exercise 2.11: Kinetic Energy of the Top

We have asserted, without proof, that the kinetic energy of the top is the kinetic energy of rotation about the pivot point. Show that this is the same as the sum of the rotational kinetic energy about its center of mass and the kinetic energy of the motion of the center of mass.

Exercise 2.12: Nutation of the Top

a. Carry out the algebra to obtain the energy (2.66) in terms of θ and $\dot{\theta}$.

b. Numerically integrate the ordinary differential equation for θ to obtain Figure (2.6).

Exercise 2.13: Precession of the Top

Consider a top that is rotating so that θ is constant.

a. Using the angular momentum integrals, compute the rate of precession $\dot{\varphi}$.

b. Assume that $\dot{\psi}$ is very large. Develop an approximate formula for the precession rate by equating the rate of change of the angular momentum to the gravitational torque on the center of mass.

c. Numerically integrate the top and check your estimate. Investigate how the rate of precession varies with θ keeping other inputs fixed.

2.11 Spin-Orbit Coupling

The rotation of planets and natural satellites is affected by the gravitational forces from other celestial bodies. As an extended application of our development of the equations governing the motion of forced rigid bodies we consider the rotation of celestial objects subject to gravitational forces.

We first develop the form of the potential energy for the gravitational interaction of an extended body with an external point mass. With this potential energy and the usual rigid body kinetic energy we can form Lagrangians that model a number of systems. We will take an initial look at the rotation of the Moon and Mercury; later, we will return to study these systems after we have developed more tools.

2.11.1 Development of the Potential Energy

The first task is to develop convenient expressions for the gravitational potential energy of the interaction of a rigid body with a distant mass point. A rigid body can be thought of as made of a large number of mass elements, subject to rigid coordinate constraints. We have seen that the kinetic energy of a rigid body is conveniently expressed in terms of the moments of inertia of the body and the angular velocity vector, which in turn can be represented in terms of a suitable set of generalized coordinates. The potential energy can be developed in a similar manner. We first represent the potential energy in terms of moments of the mass distribution and later introduce generalized coordinates as particular parameters of the potential energy.

The gravitational potential energy of a mass point and a rigid body (see Figure 2.10) is the sum of the potential energy of the mass point with each mass element of the body:

$$-\sum_{\alpha} \frac{GM'm_\alpha}{r_\alpha} \qquad (2.67)$$

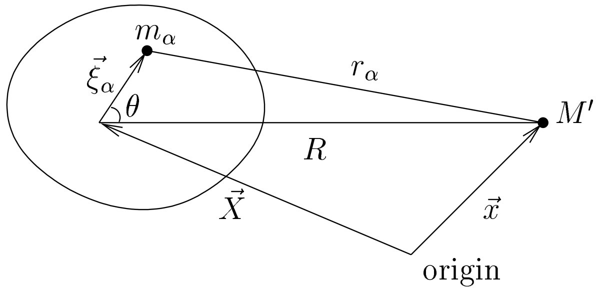

Figure 2.10 The gravitational potential energy of a mass point and a rigid body is the sum of the gravitational potential energy of the mass point with each constituent mass element of the rigid body.

where M' is the mass of the external point mass, r_α is the distance between the point mass and the constituent mass element with index α, m_α is the mass of this constituent element, and G is the gravitational constant. Let R be the distance of the center of mass of the rigid body to the point mass; R is the magnitude of the vector $\vec{x} - \vec{X}$, where the external mass point has position $\vec{x}$, and the center of mass has position $\vec{X}$. The vector from the center of mass to the constituent with index α is $\vec{\xi}_\alpha$, and has magnitude ξ_α. The distance r_α is then given by the law of cosines $r_\alpha^2 = R^2 + \xi_\alpha^2 - 2\xi_\alpha R \cos\theta_\alpha$ where θ_α is the angle between $\vec{x} - \vec{X}$ and $\vec{\xi}_\alpha$. The potential energy is then

$$-GM' \sum_\alpha \frac{m_\alpha}{(R^2 + \xi_\alpha^2 - 2\xi_\alpha R \cos\theta_\alpha)^{1/2}}. \tag{2.68}$$

This is complete, but we need to find a representation that does not mention each constituent.

Typically, the size of celestial bodies is small compared to the separation between them. We can make use of this to find a more compact representation of the potential energy. If we expand the potential energy in the small ratio ξ_α / R we find

$$-GM' \sum_\alpha m_\alpha \frac{1}{R} \sum_l \frac{\xi_\alpha^l}{R^l} P_l(\cos\theta_\alpha), \tag{2.69}$$

where P_l is the lth Legendre polynomial.[15] Interchanging the order of the summations:

$$-\frac{GM'}{R}\sum_l\sum_\alpha m_\alpha\frac{\xi_\alpha^l}{R^l}P_l(\cos\theta_\alpha). \tag{2.70}$$

Successive terms in this expansion of the potential energy typically decrease very rapidly because celestial bodies are small compared to the separation between them. We can compute an upper bound to the size of these terms by replacing each factor in the sum over α by an upper bound. The Legendre polynomials all have magnitudes less than one for arguments in the range -1 to 1. The distances ξ_α are all less than some maximum extent of the body $\xi_{\max}$. The sum over m_α times these upper bounds is just M times the upper bounds. Thus

$$\|\sum_\alpha m_\alpha\frac{\xi_\alpha^l}{R^l}P_l(\cos\theta_\alpha)\| \le M\frac{\xi_{\max}^l}{R^l}. \tag{2.71}$$

We see that the upper bound on successive terms decreases by a factor $\xi_{\max}/R$. Successive terms may be smaller still. For large bodies the gravitational force is strong enough to overcome the internal material strength of the body, so the body, over time, becomes nearly spherical. Successive terms in the expansion of the potential are measures of the deviation of the mass distribution from a spherical mass distribution. Thus for large bodies the higher order terms are small because the bodies are nearly spherical.

Consider the first few terms in l. For $l = 0$ the sum over α just gives the total mass M of the rigid body. For $l = 1$ the sum over α is zero, as a consequence of choosing the origin of the $\vec{\xi}_\alpha$ to be the center of mass. For $l = 2$ we have to do a little more work. The sum involves second moments of the mass distribution, and can be written in terms of moments of inertia of the rigid body:

$$\sum_\alpha m_\alpha\xi_\alpha^2P_2(\cos\theta_\alpha) = \sum_\alpha m_\alpha\xi_\alpha^2\left(\frac{3}{2}(\cos\theta_\alpha)^2-\frac{1}{2}\right)$$

---

[15]The Legendre polynomials may be obtained by expanding $(1+y^2-2yx)^{-1/2}$ as a power series in y. The coefficient of y^l is $P_l(x)$. The first few Legendre polynomials are:$P_0(x) = 1$, $P_1(x) = x$, $P_2(x) = \frac{3}{2}x^2-\frac{1}{2}$, and so on. The rest satisfy the recurrence relation: $lP_l(x) = (2l-1)xP_{l-1}(x)-(l-1)P_{l-2}(x)$.

$$
\begin{aligned}
&= \sum_\alpha m_\alpha \xi_\alpha^2 \left(1 - \frac{3}{2}(\sin\theta_\alpha)^2\right) \\
&= \frac{1}{2}\left(A + B + C - 3I\right),
\end{aligned}
\tag{2.72}
$$

where A, B, and C are the principal moments of inertia, and I is the moment of inertia of the rigid body about the line between the center of mass of the body to the external point mass. The moment I depends on the orientation of the rigid body relative to the line between the bodies. The contributions to the potential energy up to $l = 2$ are then[16]

$$
-\frac{GMM'}{R} - \frac{GM'}{2R^3}(A + B + C - 3I). \tag{2.73}
$$

Let $\alpha = \cos\theta_a$, $\beta = \cos\theta_b$, and $\gamma = \cos\theta_c$ be the direction cosines of the angles θ_a, θ_b and θ_c between the principal axes $\hat{a}$, $\hat{b}$, and $\hat{c}$ and the line between the center of mass and the point mass.[17] A little algebra shows $I = \alpha^2 A + \beta^2 B + \gamma^2 C$. The potential energy is then

$$
-\frac{GMM'}{R} - \frac{GM'}{2R^3}[(1 - 3\alpha^2)A + (1 - 3\beta^2)B + (1 - 3\gamma^2)C]. \tag{2.74}
$$

This is a good first approximation to the potential energy of interaction for most situations in the solar system; if we intended to land on the moon we probably would want to take into account higher order terms in the expansion.

Exercise 2.14:

a. Fill in the details that show that the sum over consitutents in equation (2.72) can be expressed as written in terms of moments of inertia. In particular, show that

$$
\sum_\alpha m_\alpha \xi_\alpha \cos\theta_\alpha = 0,
$$

$$
\sum_\alpha m_\alpha \xi_\alpha^2 = 2(A + B + C),
$$

[16] This approximate representation of the potential energy is sometimes called MacCullagh's formula.

[17] Watch out, we just reused α. It was also used as the constituent index.

and that

$$\sum_\alpha m_\alpha \xi_\alpha^2 (\sin\theta_\alpha)^2 = I.$$

b. Show that if the principal moments of inertia of a rigid body are A, B, and C, then the moment of inertia about an axis that goes through the center of mass of the body with direction cosines α, β, and γ relative to the principal axes is

$$I = \alpha^2 A + \beta^2 B + \gamma^2 C.$$

2.11.2 Rotation of the Moon and Hyperion

The approximation to the potential energy that we have derived can be used for a number of different problems. For instance, it can be used to investigate the effect of oblateness on the evolution of an artificial satellite about the Earth, or to incorporate the effect of planetary oblateness on the evolution of the orbits of natural satellites, such as the Moon, or the Galilean satellites of Jupiter. However, as the principal application here, we will use it to investigate the rotational dynamics of natural satellites and planets.

The potential energy depends on the position of the point mass relative to the rigid body and on the orientation of the rigid body. Thus the changing orientation is coupled to the orbital evolution; each affects the other. However, in many situations, the effect of the orientation of the body on the evolution of the orbit may be ignored. One way to see this is to look at the relative magnitudes of the two terms in the potential energy (2.74). We already know that the second term is guaranteed to be smaller than the first by a factor of $(\xi_{\mathrm{max}}/R)^2$, but often it is much smaller still because the body involved is nearly spherical. For example, the radius of the Moon is about a third the radius of the Earth and the distance to the Moon is about 60 Earth-radii. So the second term is smaller than the first by a factor of order 10^{-4} due to the size factors. In addition the Moon is roughly spherical and for any orientation the combination $A + B + C - 3I$ is of order $10^{-4}C$. Now C is itself of order $\frac{2}{5}MR^2$, because the density of the Moon does not vary strongly with radius. So for the Moon the second term is of order 10^{-8} relative to the first. Even radical changes in the orientation of the Moon would have little dynamical effect on the orbit of the Moon.

We can learn some important qualitative aspects of the orientation dynamics by studying a simplified model problem. First, we assume that the body is rotating about its largest moment of inertia. This is a natural assumption. Remember that for a free rigid body the loss of energy while conserving angular momentum leads to rotation about the largest moment of inertia. This is observed for most bodies in the solar system. Next, we assume that the spin axis is perpendicular to the orbital motion. This is a good approximation for the rotation of natural satellites, and is a natural consequence of tidal friction — dissipative solid body tides raised on the satellite by the gravitational interaction with the planet. Finally, for simplicity we take the rigid body to be moving on a fixed elliptic orbit. This may approximate the motion of some physical systems, provided the timescale of the evolution of the orbit is large compared to any timescale associated with the rotational dynamics that we are investigating. So we have a nice toy problem. This problem has been used to investigate the rotational dynamics of Mercury, the Moon, and other natural satellites. It makes specific predictions concerning the rotation of Phobos, a satellite of Mars, which can be compared with observations. It provides a basic understanding of the fact that Mercury rotates precisely 3 times for every 2 orbits it completes, and is the starting point for understanding the chaotic tumbling of Saturn's satellite Hyperion.

We are assuming that the orbit does not change or precess. The orbit is an ellipse with the point mass at a focus of the ellipse. The angle f (see figure 2.11) measures the position of the rigid body in its orbit relative to the point in the orbit at which the two bodies are closest.[18] We assume the orbit is a fixed ellipse, so the angle f and the distance R are periodic functions of time, with period equal to the orbit period. With the spin axis constrained to be perpendicular to the orbit plane, the orientation of the rigid body is specified by a single degree of freedom: the orientation of the body about the spin axis. We specify this orientation by the generalized coordinate θ that measures the angle to the $\hat{a}$ principal axis from the same line as we measure f, the line through the point of closest approach.

[18] Traditionally, the point in the orbit at which the two bodies are closest is called the *pericenter*, and the angle f is called the *true anomaly*.

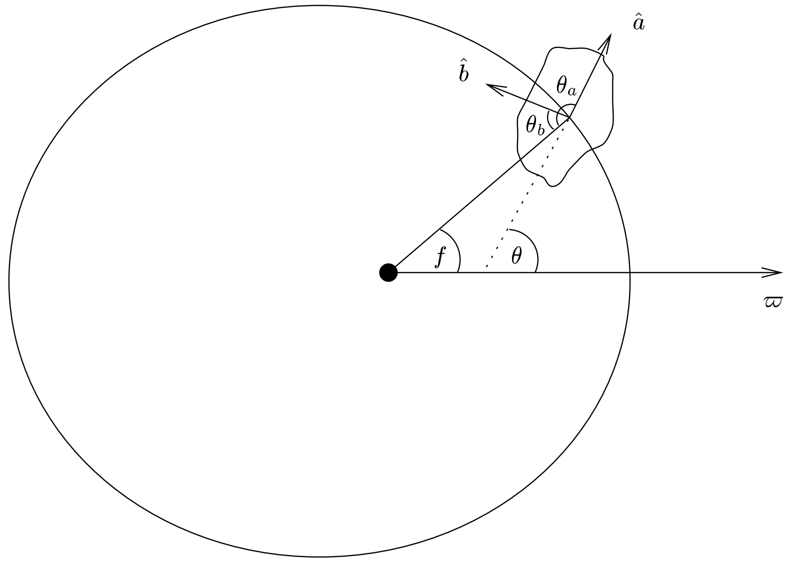

Figure 2.11 The spin-orbit model problem in which the spin axis is constrained to be perpendicular to the orbit plane has a single degree of freedom, the orientation of the body in the orbit plane. Here the orientation is specified by the generalized coordinate θ.

Having specified the coordinate system, we can work out the details of the kinetic and potential energies, and thus find the Lagrangian. The kinetic energy is

$$T(t, \theta, \dot{\theta}) = \tfrac{1}{2} C \dot{\theta}^2, \tag{2.75}$$

where C is the moment of inertia about the spin axis, and the angular velocity of the body about the $\hat{c}$ axis is $\dot{\theta}$. There is no component of angular velocity on the other principal axes.

To get an explicit expression for the potential energy we must write the direction cosines in terms of θ and f: $\alpha = \cos\theta_a = -\cos(\theta - f)$, $\beta = \cos\theta_b = \sin(\theta - f)$, and $\gamma = \cos\theta_c = 0$ because the $\hat{c}$ axis is perpendicular to the orbit plane. The potential energy is then

$$-\frac{GMM'}{R}$$
$$\quad - \frac{1}{2}\frac{GM'}{R^3}\left[(1 - 3\cos^2(\theta - f))A + (1 - 3\sin^2(\theta - f))B + C\right].$$

Since we are assuming that the orbit is given, we only need to keep terms that depend on θ. Expanding the squares of the cosine and the sine in terms of the double angles, and dropping all the terms that do not depend on θ we find the potential energy for the orientation[19]

$$V(t,\theta,\dot{\theta}) = -\frac{3}{4}\frac{GM'}{R^3(t)}(B-A)\cos 2(\theta - f(t)). \tag{2.76}$$

A Lagrangian for the model spin-orbit coupling problem is then $L = T - V$:

$$L(t,\theta,\dot{\theta}) = \frac{1}{2}C\dot{\theta}^2 + \frac{3}{4}\frac{GM'}{R^3(t)}(B-A)\cos 2(\theta - f(t)). \tag{2.77}$$

We introduce the dimensionless "out-of-roundness" parameter

$$\epsilon = \sqrt{\frac{3(B-A)}{C}}, \tag{2.78}$$

and use the fact that the orbit frequency n satisfies Kepler's third law $n^2a^3 = G(M+M')$, which is approximately $n^2a^3 = GM'$ for a small body in orbit around a much more massive one ($M \ll M'$). In terms of ϵ and n the spin-orbit Lagrangian is

$$L(t,\theta,\dot{\theta}) = \frac{1}{2}C\dot{\theta}^2 + \frac{n^2\epsilon^2 C}{4}\frac{a^3}{R^3(t)}\cos 2(\theta - f(t)). \tag{2.79}$$

This is a problem with one degree of freedom with terms that vary periodically with time.

The Lagrange equations are derived in the usual manner. The equations are

$$CD^2\theta(t) = -\frac{n^2\epsilon^2 C}{2}\frac{a^3}{R^3(t)}\sin 2(\theta(t) - f(t)). \tag{2.80}$$

The equation of motion is very similar to that of the periodically driven pendulum. The main difference here is that not only is the strength of the acceleration changing periodically, but in the spin-orbit problem the center of attraction is also varying periodically.

---

[19] The given potential energy differs from the actual potential energy in that non-constant terms that do not depend on θ and consequently do not affect the evolution of θ have been dropped.

We can give a physical interpretation of this equation of motion. It states that the rate of change of the angular momentum is equal to the applied torque. The torque on the body arises because the body is out of round and the gravitational force varies as the inverse square of the distance. Thus the force per unit mass on the near side of the body is stronger than the acceleration of the body as a whole, and the force per unit mass on the far side of the body is a little less than the acceleration of the body as a whole. Thus, relative to the acceleration of the body as a whole the far side is forced outward while the inner part of the body is forced inward. The net effect is a torque on the body, which tries to align the long axis of the body with the line to the external point mass. If θ is a bit larger than f then there is a negative torque, and if θ is a bit smaller than f then there is a positive torque, both of which would align the long axis with the planet if given a fair chance. The torque arises because of the difference of the inverse R^2 force across the body, so the torque is proportional to R^{-3}. There is only a torque if the body is out-of-round, for otherwise there is no handle to pull on. This is reflected in the factor $B - A$, which appears in the expression for the torque. The potential depends only on the moment of inertia, thus the body has the same dynamics if it is rotated by 180°. The factor of 2 in the argument of sine reflects this symmetry. This torque is called the "gravity gradient torque."

To compute the evolution requires a bunch of detailed preparation similar to what has been done for other problems. There are many interesting phenomena to explore. We can take parameters appropriate for the Moon, and find that Mr. Moon does not constantly point the same face to the Earth, but instead constantly shakes his head in dismay at what goes on here. If we nudge the Moon a bit, say by hitting it with an asteroid, we find that the long axis oscillates back and forth with respect to the direction that points to the Earth. For the Moon, the orbital eccentricity is currently about 0.05, and the out-of-roundness parameter is about $\epsilon = 0.026$. Figure (2.12) shows the angle $\theta - f$ as a function of time for two different values of the "lunar" eccentricity. The plot spans 50 lunar orbits, or a little under 4 years. This Moon has been kicked by a large asteroid and has initial rotational angular velocity $\dot{\theta}$ equal to 1.01 times the orbit frequency. The initial orientation is $\theta = 0$. The smooth trace shows the evolution if the orbital eccentricity is set to zero. We see an oscillation with a period of about 40 lunar orbit periods or about 3 years. The more wiggly trace shows the evolution of $\theta - f$ with an orbital eccentricity of 0.05, near the current lunar eccentricity. The lunar eccentricity superimposes an apparent shaking of the face of the moon back and forth with the period of the lunar orbit. Though the Moon does slightly change its rate of rotation during the course of its orbit, most of this shaking is due to the non-uniform motion of the Moon in its elliptical orbit. This oscillation is called the "optical libration of the Moon," and it allows us to see a bit more than half the surface of the Moon. The longer period oscillation induced by the kick is called the "free libration of the Moon." It is "free" because we are free to excite it by choosing appropriate initial conditions. The mismatch of the orientation of the moon caused by the optical libration actually produces a periodic torque on the Moon, which slightly speeds up and slows down the Moon during every orbit. The resulting oscillation is called the "forced libration of the Moon," but it is too small to see in this plot.

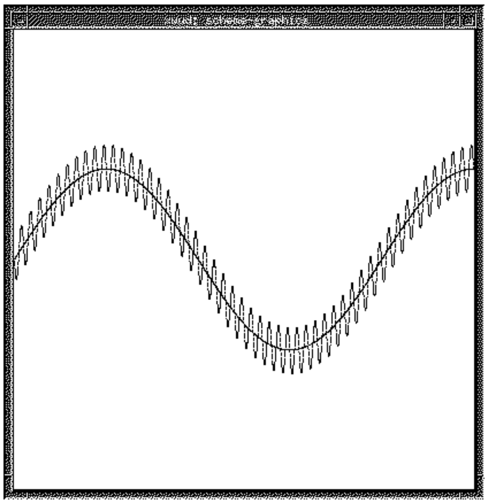

Figure 2.12 The angle $\theta - f$ versus time for 50 orbit periods. The ordinate scale is ± 1 radian. The Moon has been kicked so that the initial rotational angular velocity is 1.01 times the orbital frequency. The trace with fewer wiggles was computed with zero lunar orbital eccentricity; the other trace was computed with lunar orbital eccentricity of 0.05. The period of the rapid oscillations is the lunar orbit period, and are due mostly to the non-uniform motion of f.

The oscillation period of the free libration is easily calculated. We see that the eccentricity of the orbit does not substantially affect the period, so consider the special case of zero eccentricity. In this case $R = a$, a constant, and $f(t) = nt$ where n is the orbital frequency (traditionally called the *mean motion*). The equation of motion becomes

$$D^2\theta(t) = -\frac{n^2\epsilon^2}{2}\sin 2(\theta(t) - nt). \tag{2.81}$$

Let $\varphi(t) = \theta(t) - nt$, and consequently $D\varphi = D\theta - n$, and $D^2\varphi = D^2\theta$. Substituting these, the equation governing the evolution of φ is

$$D^2\varphi = -\frac{n^2\epsilon^2}{2}\sin 2\varphi. \tag{2.82}$$

For small deviations from synchronous rotation (small φ) this is

$$D^2\varphi = -n^2\epsilon^2\varphi, \tag{2.83}$$

so we see that the small amplitude oscillation frequency of φ is $n\epsilon$. For the Moon, ϵ is about 0.026, so the period is about 1/0.026 orbit periods or about 40 lunar orbit periods, which is what we observed.

It is perhaps more fun to see what happens if the out-of-roundness parameter is large. After our experience with the driven pendulum it is no surprise that we find abundant chaos in the spin-orbit problem when the system is strongly driven by having large ϵ and significant e. There is indeed one body in the solar system that exhibits chaotic rotation — Hyperion, a small satellite of Saturn. Though our model is not adequate for a complete account of Hyperion, we can show that our toy model exhibits chaotic behavior for parameters appropriate for Hyperion. We take $\epsilon = 0.89$ and $e = 0.1$. Figure (2.13) shows $\theta - f$ for 50 orbits, starting with $\theta = 0$ and $\dot{\theta} = 1.05$. We see that sometimes one face of the body oscillates facing the planet, sometimes the other face oscillates facing the planet, and sometimes the body rotates relative to the planet in either direction.

If we were to relax our restriction that the spin axis is fixed perpendicular to the orbit, then we find that the Moon maintains this orientation of the spin axis even if nudged a bit, but for Hyperion the spin axis almost immediately falls away from this configura-

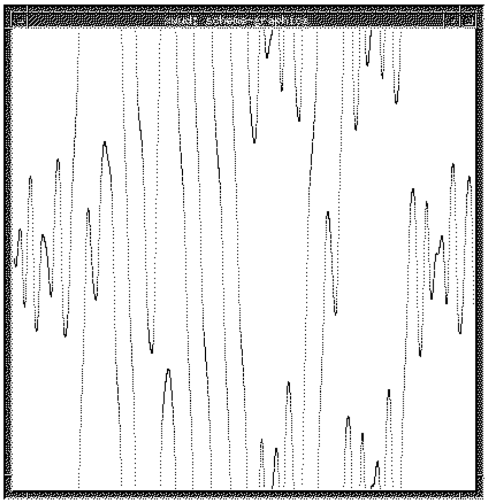

Figure 2.13 The angle $\theta - f$ versus time for 50 orbit periods. The ordinate scale is $\pm\pi$ radian. The out-of-roundness parameter is large $\epsilon = 0.89$, with an orbital eccentricity of $e = 0.1$. The system is strongly driven. The rotation is apparently chaotic.

tion. The state in which Hyperion on average points one face to Saturn is dynamically unstable to chaotic tumbling. Observations of Hyperion confirm that Hyperion is chaotically tumbing.

2.12 Euler's Equations for a Free Rigid Body

For a free rigid body we have seen that the components of the angular momentum on the principal axes comprise a self contained dynamical system: the variation of the principal axis components depends only on the principal axis components. Here we derive equations that govern the evolution of these components.

The starting point for the derivation is the conservation of the vector angular momentum. The components of the angular momentum on the principal axes are

$$\mathbf{L}' = \mathbf{I}'\boldsymbol{\omega}' \tag{2.84}$$

where $\boldsymbol{\omega}'$ is composed of the components of the angular velocity vector on the principal axes, and $\mathbf{I}'$ is the matrix representation of the inertia tensor with respect to the principal axis basis:

$$\mathbf{I}' = \begin{bmatrix} A & 0 & 0 \\ 0 & B & 0 \\ 0 & 0 & C \end{bmatrix}. \tag{2.85}$$

The body components of the angular momentum $\mathbf{L}'$ are related to the components $\mathbf{L}$ on the fixed rectangular basis $\hat{e}_i$ by

$$\mathbf{L} = \mathbf{M}\mathbf{L}', \tag{2.86}$$

where $\mathbf{M}$ is the matrix representation of the rotation that carries the body and all vectors attached to the body from the reference orientation of the body to the actual orientation.

The vector angular momentum is conserved for free rigid body motion, and so are its components on a fixed rectangular basis. So, along solution paths

$$0 = D\mathbf{L} = D\mathbf{M}\,\mathbf{L}' + \mathbf{M}\,D\mathbf{L}'. \tag{2.87}$$

Solving, we find

$$D\mathbf{L}' = -\mathbf{M}^{\mathrm{T}}\,D\mathbf{M}\,\mathbf{L}'. \tag{2.88}$$

In terms of $\boldsymbol{\omega}'$ this is

$$\begin{aligned} \mathbf{I}'D\boldsymbol{\omega}' &= -\mathbf{M}^{\mathrm{T}}\,D\mathbf{M}\,\mathbf{I}'\boldsymbol{\omega}' \\ &= -\mathbf{M}^{\mathrm{T}}\,\mathsf{A}(\mathbf{M}\boldsymbol{\omega}')\,\mathbf{M}\,\mathbf{I}'\boldsymbol{\omega}', \end{aligned} \tag{2.89}$$

where we have used Equation (2.38) to write $D\mathbf{M}$ in terms of A. The function A has the property[20]

$$\mathbf{R}^{\mathrm{T}}\,\mathsf{A}(\mathbf{R}\mathbf{v})\,\mathbf{R} = \mathsf{A}(\mathbf{v}) \tag{2.90}$$

[20]Rotating the cross product of two vectors gives the same vector that is obtained by taking the cross product of two rotated vectors: $R(\vec{u} \times \vec{v}) = (R\vec{u}) \times (R\vec{v})$.

for any vector with components $\mathbf{v}$ and any rotation with matrix representation $\mathbf{R}$. Using this property of A we find *Euler's equations*:

$$\mathbf{I}' D\boldsymbol{\omega}' = -\mathsf{A}(\boldsymbol{\omega}')\,\mathbf{I}'\boldsymbol{\omega}'. \tag{2.91}$$

Euler's equations give the time derivative of the body components of the angular velocity vector entirely in terms of the components of the angular velocity vector and the principal moments of inertia. Let ω^a, ω^b, and ω^c denote the components of the angular velocity vector on the principal axes. Then Euler's equations can be written as the component equations

$$\begin{aligned} A\,D\omega^a &= (B - C)\,\omega^b\omega^c \\ B\,D\omega^b &= (C - A)\,\omega^c\omega^a \\ C\,D\omega^c &= (A - B)\,\omega^a\omega^b. \end{aligned} \tag{2.92}$$

Alternately, we can rewrite Euler's equations in terms of the components of the angular momentum on the principal axes

$$D\mathbf{L}' = -\mathsf{A}((\mathbf{I}')^{-1}\mathbf{L}')\mathbf{L}'. \tag{2.93}$$

These equations confirm that the time derivatives of the components of the angular momentum on the principal axes depend only on the components of the angular momentum on the principal axes.

Euler's equations are very simple, but they do not completely determine the evolution of a rigid body — they do not give the spatial orientation of the body. However, equation (2.38) and property (2.90) can be used to relate the derivative of the orientation matrix to the body components of the angular velocity vector:

$$D\mathbf{M} = \mathbf{M}\mathsf{A}(\boldsymbol{\omega}'). \tag{2.94}$$

A straightforward method of using these equations is to integrate them componentwise as a set of nine first order ordinary differential equations, with initial conditions determining the initial configuration matrix. Together with Euler's equations, which describe how the body components of the angular velocity vector change with time, this system of equations governing the motion of a rigid body is complete. However, the reader will no doubt have noticed that this approach is rather wasteful. The fact that the orientation matrix can be specified with only three parameters has not been taken into account. We should be integrating three equations for the orientation, given $\boldsymbol{\omega}'$, not nine. To accomplish this we once again need to parameterize the configuration matrix.

For example, we can use Euler angles to parameterize the orientation:

$$\mathsf{M}(\theta, \varphi, \psi) = \mathbf{R}_z(\varphi)\mathbf{R}_x(\theta)\mathbf{R}_z(\psi). \tag{2.95}$$

We form $\mathbf{M}$ by composing M with an Euler coordinate path. Equation (2.94) can then be used to solve for $D\theta$, $D\varphi$, and $D\psi$. We find

$$\begin{bmatrix} D\theta \\ D\varphi \\ D\psi \end{bmatrix} = \frac{1}{\sin\theta} \begin{bmatrix} \cos\psi\sin\theta & -\sin\psi\sin\theta & 0 \\ \sin\psi & \cos\psi & 0 \\ -\sin\psi\cos\theta & \cos\psi\cos\theta & \sin\theta \end{bmatrix} \begin{bmatrix} \omega^a \\ \omega^b \\ \omega^c \end{bmatrix}. \tag{2.96}$$

This gives us the desired equation for the orientation. Note that it is singular for $\theta = 0$ as are Lagrange's equations. So Euler's equations using Euler angles for the configuration have the same problem as did the Lagrange equations using Euler angles. Again, this is a manifestation of the fact for $\theta = 0$ the orientation depends only on $\varphi + \psi$. The singularity in the equations of motion for $\theta = 0$ does not correspond to anything funny in the motion of the rigid body. A practical solution to the singularity problem is to choose another set of Euler-like angles that have a singularity in a different place, and switch from one to the other when the going gets tough.

Exercise 2.15:

Fill in the details of the derivation of equation (2.96). You may want to use the computer to help with the algebra.

2.12.1 Euler's Equations for Forced Rigid Bodies

Euler's equations were derived for a free rigid body. In general, we must be able to deal with external forcing. How do we do this? First, we derive expressions for the vector torque. Then we include the vector torque in the Euler equations.

We derive the vector torque in a manner analogous to the derivation of the vector angular momentum. That is, we derive one component and then argue that since the coordinate system is arbitrary, all components have the same form.

Suppose we have a rigid body subject to some potential energy that depends only on time and the configuration. A Lagrangian is $L = T - V$. If we use the Euler angles as generalized coordinates, the last of the three active Euler rotations that define the orientation is a rotation about the $\hat{z}$ axis. The magnitude of this rotation is given by the angle φ. The Lagrange equation for φ gives[21]

$$Dp_\varphi(t) = -\partial_{1,1}V(t; \theta(t), \varphi(t), \psi(t)). \tag{2.97}$$

If we define T_z, the component of the torque about the z axis, to be minus the derivative of the potential energy with respect to the angle of rotation of the body about the z axis,

$$T_z(t) = -\partial_{1,1}V(t; \theta(t), \varphi(t), \psi(t)), \tag{2.98}$$

then we see that

$$T_z(t) = Dp_\varphi(t). \tag{2.99}$$

We have already identified the momentum conjugate to φ as one component, L_z, of the vector angular momentum $\vec{L}$ (see section 2.9), so

$$T_z = DL_z(t). \tag{2.100}$$

Since the orientation of the reference rectangular basis vectors is arbitrary we may choose them any way that we please. Thus if we want any component of the vector torque, we may choose the z-axis so that we can compute it in this way. We can conclude that the vector torque gives the rate of change of the vector angular momentum

$$D\vec{L} = \vec{T}. \tag{2.101}$$

[21] In this equation we have a partial derivative with respect to a component of the coordinate argument of the potential energy function. The first subscript on the ∂ symbol indicates the coordinate argument. The second one selects the φ component.

Having obtained a general prescription for the vector torque, we address how the vector torque may be included in Euler's equations. Euler's equations expressed the fact that the vector angular momentum is conserved. Let's return to that calculation, but now include a torque with components $\mathbf{T}$

$$D\mathbf{L} = \mathbf{T} = D\mathbf{M}\,\mathbf{L}' + \mathbf{M}\,D\mathbf{L}'. \tag{2.102}$$

Carrying out the same steps as before we find

$$D\mathbf{L}' + \mathsf{A}((\mathbf{I}')^{-1}\mathbf{L}')\mathbf{L}' = \mathbf{M}^{-1}\mathbf{T} = \mathbf{T}', \tag{2.103}$$

where the components of the vector torque on the principal axes are:

$$\mathbf{T}' = \mathbf{M}^{-1}\mathbf{T}. \tag{2.104}$$

In terms of $\boldsymbol{\omega}$ this is

$$\mathbf{I}'D\boldsymbol{\omega}' + \mathsf{A}(\boldsymbol{\omega}')\,\mathbf{I}'\boldsymbol{\omega}' = \mathbf{T}'. \tag{2.105}$$

In components,

$$A\,D\omega^a - (B - C)\,\omega^b\omega^c = T^a \tag{2.106}$$
$$B\,D\omega^b - (C - A)\,\omega^c\omega^a = T^b \tag{2.107}$$
$$C\,D\omega^c - (A - B)\,\omega^a\omega^b = T^c. \tag{2.108}$$

Note that the torque entered only the equations for the body angular momentum or alternately for the body angular velocity vector. When written in terms of the angular velocity vector, the equations governing the orientation are not modified by the torque. In a sense, Euler's equations contain the dynamics, and the equations governing the orientation are kinematic. Of course, Lagrange's equations must be modified by the potential that gives rise to the torques; in this sense Lagrange's equations contain both dynamics and kinematics.

2.13 Non-singular Generalized Coordinates

The Euler angles provide a convenient way to parameterize the orientation of a rigid body. However, the equations of motion derived for them have singularities. Though we can avoid the singularities by using other Euler-like combinations with different singularities, this kludge is not very satisfying. Let's brainstorm a bit and see if we can come up with something better.

What does it take to specify an orientation? Perhaps we can take a hint from Euler's theorem. Recall that Euler's theorem states that any orientation can be reached with a single rotation. So one idea to specify the orientation of a body is to parameterize this single rotation that does the job. To specify this rotation we need to specify the rotation axis and the amount of rotation. We contrast this with the Euler angles that specify three successive rotations. These three rotations need not have any relation to the single composite rotation that gives the orientation. Isn't it curious that the Euler angles make no use of Euler's theorem?

We can think of several ways of specifying a rotation. One way would be to specify the rotation axis by the latitude and the longitude that the rotation axis pierces a sphere. The amount of rotation needed to take the body from the reference position could be specified by one more angle. We can predict though that this choice of coordinates will have similar problems to those of the Euler angles: if the amount of rotation is zero, then the latitude and longitude of the rotation axis is undefined. So the Lagrange equations for these angles are probably singular. Another idea, without this defect, is to represent the rotation by the rectangular components of an orientation vector $\vec{o}$; we take the direction of the orientation vector to be the same as the axis of rotation that takes the body from the reference orientation to the present orientation, and the length of the orientation vector is the angle by which the body must be rotated, in a right-hand sense about the orientation vector. With this choice of coordinates, if the angle of rotation is zero then the length of the vector is zero and has no unwanted direction. This choice looks promising.

We denote the rectangular components of $\vec{o}$ by (o_x, o_y, o_z); these are our generalized coordinates. The magnitude $o = \sqrt{o_x^2 + o_y^2 + o_z^2}$ is the angle of rotation. The axis of the rotation is $\hat{o} = \vec{o}/o$. We denote the components of $\hat{o}$ by $\hat{o}_x$, $\hat{o}_y$, and $\hat{o}_z$. The first step in implementing the components of the orientation vector as generalized coordinates is to construct the rotation M to which the orientation vector $\vec{o}$ corresponds. Let $\vec{u}'$ be a vector to one of the constituents of the body in the reference orientation, and $\vec{u}$ be the vector to that constituent after rotation by M:

$$\vec{u} = M\vec{u}'. \tag{2.109}$$

We can determine M by considering how the rotation represented by $\vec{o}$ affects the vector $\vec{u}'$. The component of $\vec{u}'$ parallel to $\vec{o}$ is unaffected. The perpendicular component is reduced by the cosine of the rotation angle, and a component perpendicular to these two is generated that is proportional to the sine of the rotation angle and the magnitude of the perpendicular component. Let $(\vec{u}')^{\|} = (\vec{u}' \cdot \hat{o})\hat{o}$ and $(\vec{u}')^{\perp} = \vec{u}' - (\vec{u}')^{\|}$, then

$$\vec{u} = (\vec{u}')^{\|} + (\vec{u}')^{\perp} \cos o + \hat{o} \times (\vec{u}')^{\perp} \sin o. \tag{2.110}$$

From this expression we can construct the equivalent rotation matrix. First define some useful primitive matrices:

$$\mathbf{A} = \mathsf{A}(\hat{o}) = \begin{bmatrix} 0 & -\hat{o}_z & \hat{o}_y \\ \hat{o}_z & 0 & -\hat{o}_x \\ -\hat{o}_y & \hat{o}_x & 0 \end{bmatrix}, \tag{2.111}$$

and

$$\mathbf{S} = \begin{bmatrix} \hat{o}_x^2 & \hat{o}_x\hat{o}_y & \hat{o}_x\hat{o}_z \\ \hat{o}_x\hat{o}_y & \hat{o}_y^2 & \hat{o}_y\hat{o}_z \\ \hat{o}_x\hat{o}_z & \hat{o}_y\hat{o}_z & \hat{o}_z^2 \end{bmatrix}, \tag{2.112}$$

with the identity

$$\mathbf{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{2.113}$$

The matrix $\mathbf{A}$ is antisymmetric and $\mathbf{S}$ is the symmetric outer product of the components of $\hat{o}$. The matrix $\mathbf{A}$ implements the cross product of $\hat{o}$ with other vectors, and the matrix $\mathbf{S}$ projects vectors to the orientation vector. We have the following identities:

$$\mathbf{AA} = \mathbf{S} - \mathbf{I} \tag{2.114}$$

$$\mathbf{SS} = \mathbf{S} \tag{2.115}$$

$$\mathbf{SA} = \mathbf{0} \tag{2.116}$$

$$\mathbf{AS} = \mathbf{0}. \tag{2.117}$$

In terms of these matrices, the rotation matrix is

$$\mathbf{M} = \mathbf{I}\cos o + \mathbf{A}\sin o + \mathbf{S}(1 - \cos o) \tag{2.118}$$

The inverse of a rotation is a rotation about the same axis but by the negative of the rotation angle. Thus the inverse of $\mathbf{M}$ can be written down immediately

$$\mathbf{M}^{-1} = \mathbf{I}\cos o - \mathbf{A}\sin o + \mathbf{S}(1 - \cos o). \tag{2.119}$$

We verify that the inverse of the rotation matrix is the transpose of the rotation matrix by recalling that $\mathbf{I}$ and $\mathbf{S}$ are symmetric and $\mathbf{A}$ is antisymmetric.

The computation of the angular velocity vector from $\mathbf{M}^{\mathsf{T}}$ and $D\mathbf{M}$ is straightforward, though tedious; the angular velocity vector turns out to have a simple form:

$$\boldsymbol{\omega} = \left[\mathbf{I}\frac{\sin o}{o} + \mathbf{A}\frac{1 - \cos o}{o} + \mathbf{S}\left(1 - \frac{\sin o}{o}\right)\right] D\mathbf{o}. \tag{2.120}$$

The components of the angular velocity vector on the principal axes can be found by multiplying the above by $\mathbf{M}^{-1} = \mathbf{M}^{\mathsf{T}}$:

$$\boldsymbol{\omega}' = \left[\mathbf{I}\frac{\sin o}{o} - \mathbf{A}\frac{1 - \cos o}{o} + \mathbf{S}\left(1 - \frac{\sin o}{o}\right)\right] D\mathbf{o}. \tag{2.121}$$

Let

$$\mathbf{W} = \left[\mathbf{I}\frac{\sin o}{o} - \mathbf{A}\frac{1 - \cos o}{o} + \mathbf{S}\left(1 - \frac{\sin o}{o}\right)\right]. \tag{2.122}$$

then we have

$$\boldsymbol{\omega}' = \mathbf{W}\, D\mathbf{o}. \tag{2.123}$$

Solving, we find

$$D\mathbf{o} = \mathbf{W}^{-1}\boldsymbol{\omega}'. \tag{2.124}$$

The matrix $\mathbf{W}$ is not an orthogonal matrix, so its inverse is not trivial, but we can use the properties of the primitive matrices to find it. Suppose we have a matrix of the form

$$\mathbf{N} = a\mathbf{I} + b\mathbf{A} + c\mathbf{S} \tag{2.125}$$

that we wish to invert. Let's guess that the inverse matrix has a similar form.

$$\mathbf{N}^{-1} = a'\mathbf{I} + b'\mathbf{A} + c'\mathbf{S}. \tag{2.126}$$

We wish to find the coefficients a', b', and c' so that $\mathbf{NN}^{-1} = I$. We find three conditions on the coefficients

$$1 = aa' - bb'r^2 \tag{2.127}$$
$$0 = ab' + ba' \tag{2.128}$$
$$0 = ac' + ca' + bb' + cc'r^2, \tag{2.129}$$

with solution

$$a' = \frac{a}{a^2 + b^2} \tag{2.130}$$
$$b' = \frac{-b}{a^2 + b^2} \tag{2.131}$$
$$c' = \frac{b^2 - ac}{a^3 + a^2c + ab^2 + b^2c} \tag{2.132}$$

We can now invert the matrix $\mathbf{W}$ using its representation in terms of primitive matrices to find

$$\mathbf{W}^{-1} = \frac{1}{2}\mathbf{I}\left(\frac{o\sin o}{1-\cos o}\right) + \frac{o}{2}\mathbf{A} + \frac{1}{2}\mathbf{S}\left(2 - \frac{o\sin o}{1-\cos o}\right) \tag{2.133}$$

Note that all terms have finite limits as $o \to 0$. There is however a new singularity. As $o \to 2\pi$ two of the denominators become singular, but there the zeros in the numerators are not strong enough to kill the singularity. This is the expected singularity that corresponds to the fact that at radius 2π the orientation vector corresponds to no rotation, but nevertheless specifies a rotation axis. This singularity is easy to avoid. Whenever the orientation vector develops a magnitude larger than π simply replace it by the equivalent orientation vector $\vec{o}' = \vec{o} - 2\pi\hat{o}$.

We can write the equations governing the evolution of the orientation as a vector equation in terms of $\vec{\omega}' = M^{-1}\vec{\omega}$

$$D\vec{o} = f(o)\vec{\omega}' + \frac{1}{2}\vec{o}\times\vec{\omega}' + g(o)\vec{o}(\vec{o}\cdot\vec{\omega}') \tag{2.134}$$

with two auxilliary functions

$$f(x) = \frac{1}{2}\frac{x \sin x}{1 - \cos x} \tag{2.135}$$

$$g(x) = \frac{1 - f(x)}{x^2}. \tag{2.136}$$

The equation of motion for the orientation vector is surprisingly simple. Both auxilliary functions have finite limits at zero:

$$\lim_{x\to 0} f(x) = 1$$

$$\lim_{x\to 0} g(x) = \tfrac{1}{6}. \tag{2.137}$$

Orientation vectors with magnitude less than or equal to π are enough to specify all orientations, and the equations of motion in this region have no singularities. The orientation vector may develop magnitudes greater than π but then we replace it by the equivalent orientation vector with magnitude less than π. And there is no hurry to do this because the equations are not singular until the magnitude reaches 2π. Thus we have a complete non-singular specification of the rigid body dynamics.

A practical matter

To use the orientation vector we are presented with the practical problem of converting between the orientation vector representation of the orientation and other representations. we can consider the rotation matrix $\mathbf{M}$ as an intermediate universal representation. Whatever generalized coordinates have been chosen, we must be able to compute the rotation matrix to which the coordinates correspond. We must also solve the converse problem — the determination of the generalized coordinates from the rotation matrix.

We already have the explicit form for the rotation matrix in terms of the orientation vector in equation (2.118), repeated here for convenience,

$$\mathbf{M} = \mathbf{I}\cos o + \mathbf{A}\sin o + \mathbf{S}(1 - \cos o). \tag{2.138}$$

We can solve the inverse problem by examining this same equation. We note that of the contributions to $\mathbf{M}$ two parts are symmetric and one is antisymmetric. We can isolate the antisymmetric component by subtracting the transpose. We have

$$\mathbf{A} \sin o = \frac{1}{2} (\mathbf{M} - \mathbf{M}^\mathsf{T}) . \tag{2.139}$$

But the matrix $\mathbf{A}$ is simply related to the orientation vector

$$\mathbf{A} = \mathsf{A} \left(\frac{\mathbf{o}}{o} \right) . \tag{2.140}$$

We use the inverse operation A^{-1} that extracts the components of a 3-vector from an antisymmetric 3x3 matrix. So we have

$$\frac{\mathbf{o}}{o} = \mathsf{A}^{-1}(\mathbf{A}). \tag{2.141}$$

Note that information about the magnitude o of the rotation is not available in $\mathbf{A}$ by itself. However, the combination of $\mathbf{M}$ and its transpose produces a scaled version of $\mathbf{A}$ from which the magnitude of the rotation can be recovered

$$\frac{\sin o}{o} \mathbf{o} = \mathsf{A}^{-1} \left(\frac{1}{2} (\mathbf{M} - \mathbf{M}^\mathsf{T}) \right) . \tag{2.142}$$

The length of the vector represented by the components on the left-hand side is just $\sin o$. This does not uniquely determine o, because o spans the interval 0 to π. To completely determine o and thus $\vec{o}$ we need more information, say by determining $\cos o$. We can get $\cos o$ easily enough. Examination of the components shows

$$\cos o = \frac{1}{2} \left[\frac{1}{2} \mathrm{trace} (\mathbf{M} + \mathbf{M}^\mathsf{T}) - 1 \right] . \tag{2.143}$$

Having determined both the sine and the cosine of o we can determine o. Of course, some these expressions contain divisions by o that may be zero, but if $o = 0$ then the orientation vector is just the zero vector. This completes the solution of the practical problem of going to and from the orientation vector.

2.13.1 Composition of Rotations

We can ask the following question: "To which rotation does the composition of two rotations correspond?" Alternatively, "What is the algebra of orientation vectors?" We have all the pieces, to answer this question is just a matter of computation. Given two rotations represented by the rotation matrices $\mathbf{M}_1$ and $\mathbf{M}_2$, the rotation matrix of the composition of these rotations is $\mathbf{M} = \mathbf{M}_2\mathbf{M}_1$. Each of these rotation matrices can be converted to the equivalent orientation vector. We can define the composition $\vec{o} = \vec{o}_2 \circ \vec{o}_1$.

Let $\alpha = (\sin o)/o$, $\beta = (1 - \cos o)/o^2$, and $\gamma = \cos o$. By direct calculation we find

$$\begin{aligned}\alpha\vec{o} = \vec{o}_1 &\left\{\alpha_1\left(\frac{1+\gamma_2}{2}\right) - (\vec{o}_1 \cdot \vec{o}_2)\frac{\alpha_2\beta_1}{2}\right\}\\ &+ \vec{o}_2\left\{\alpha_2\left(\frac{1+\gamma_1}{2}\right) - (\vec{o}_1 \cdot \vec{o}_2)\frac{\alpha_1\beta_2}{2}\right\}\\ &+ (\vec{o}_1 \times \vec{o}_2)\left\{-\frac{\alpha_1\alpha_2}{2} + \frac{\beta_1\beta_2}{2}(\vec{o}_1 \cdot \vec{o}_2)\right\}\end{aligned} \tag{2.144}$$

and

$$\gamma = \frac{1}{2}(1+\gamma_1)(1+\gamma_2) - 1 + \frac{1}{2}(\vec{o}_1 \cdot \vec{o}_2)^2\beta_1\beta_2 - (\vec{o}_1 \cdot \vec{o}_2)\alpha_1\alpha_2, \tag{2.145}$$

which together determine $\vec{o}$.

Well, the formulas are rather complicated, but it turns out that with a little rearrangement they can be made quite simple. Let $c = \cos(o/2)$ and $s = \sin(o/2)$, and define $\vec{q} = (s/o)\vec{o}$. The vector $\vec{q}$ is a scaled version of $\vec{o}$; instead of having the magnitude o as $\vec{o}$ does, the vector $\vec{q}$ has the magnitude $s = \sin(o/2)$. Notice that if o is restricted to magnitudes less than π then the magnitude of the rotation o can be recovered from the magnitude of $\vec{q}$. Thus, with this restriction, the vector $\vec{q}$ corresponds to a unique rotation, no extra information is needed. Nevertheless it is convenient to keep track of the cosine of the half-angle as well as the sine; so let $q = c = \cos(o/2)$.[22] The magnitude of $\vec{q} = s$ and $q = c$, so $q^2 + \vec{q}\cdot\vec{q} = 1$. We can reexpress the formulas for the composition of two rotations in terms of $\vec{q}$ and q for each rotation. We have

$$\vec{q} = q_2\vec{q}_1 + q_1\vec{q}_2 + \vec{q}_2 \times \vec{q}_1 \tag{2.146}$$

$$q = q_1q_2 - \vec{q}_1 \cdot \vec{q}_2. \tag{2.147}$$

[22]This notation has the potential for great confusion: q is not the magnitude of the vector $\vec{q}$. Watch out!

Now that is a significant simplification! The 4-tuple formed from q with the three components of $\vec{q}$ are the components of Hamilton's *quaternion*. We see that the vector part of the quaternion that represents an orientation is a scaled version of the orientation vector.

Hamilton discovered an even more elegant way of writing the formula for the composition of two rotations. Introduce three *unit quaternions*: i, j, k, such that $i^2 = j^2 = k^2 = -1$, $ij = k$, $jk = i$, $ki = j$, and each of the unit quaternions anticommute: $ij = -ji$, and so on. Denote the three components of $\vec{q}$ by (q^1, q^2, q^3), and q by q^0. Then define the composite quaternion $\mathbf{q} = q^0 + iq^1 + jq^2 + kq^3$. With the rule for how the unit quaternions multiply, the formula for the composition of two rotations becomes simply a multiplication. The quaternions generalize the idea of complex numbers. In fact they are the only algebraically closed field besides complex numbers. The unit quaternions cannot be represented simply as real numbers or complex numbers, particularly because of their anticommuting properties. However, they do have a representation as 2x2 matrices of complex numbers. The units are

$$1 \mapsto \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{2.148}$$

$$i \mapsto \begin{bmatrix} 0 & -i \\ -i & 0 \end{bmatrix} \tag{2.149}$$

$$j \mapsto \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \tag{2.150}$$

$$k \mapsto \begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix}, \tag{2.151}$$

where the i on the right-hand side is the usual imaginary unit $i^2 = -1$. These matrices are related to the Pauli spin matrices. There are other representations, but this is carrying us too far afield.

If we are faced with the task of composing rotations repeatedly, then the quaternions will be a handy intermediate representation. The quaternions also have the advantage that we do not need to worry about whether the angle of rotation is in the appropriate range. However, the equation of motion for the orientation vector is simpler than the equation of motion for the quaternion, so we will stick with the orientation vector when we need non-singular equations of motion for the orientation.

Exercise 2.16: Composition

Verify that the rule for composition of two rotations in terms of the orientation vectors (equations 2.144 and 2.144) is equivalent to the rule for multiplying two quaterions (equation 2.147).

Exercise 2.17: Equation of Motion

Find the equation of motion for the orientation quaternion in terms of the angular velocity vector.

2.14 Summary

A rigid body is an example of a mechanical system with constraints. Thus, in a sense this chapter on rigid bodies was nothing but an extended example of the application of the ideas developed in the first chapter.

We first showed that the kinetic energy for a rigid body separates into a translational kinetic energy and a rotational kinetic energy. The center of mass plays a special role in this separation.

The rotational kinetic energy is simply expressed in terms of the inertia tensor and the angular velocity vector.

One choice for generalized coordinates is the Euler angles. They form suitable generalized coordinates, but are otherwise not special or well motivated.

Having developed the expressions for the kinetic energy that take into account the body constraints and expressed the remaining freedoms of motion in terms of suitable generalized coordinates, the equations of motion for the free rigid body are just Lagrange's equations.

The vector angular momentum is conserved if there are no external torques. The time derivative of the body components of the angular momentum can be written entirely in terms of the body components of the angular momentum, and the three principal moments of inertia. The body components of angular momentum form a self-contained dynamical sub-system.

The Lagrange equations for the Euler angles are singular for some Euler angles. Other choices of generalized coordinates like the Euler angles have similar problems. Equations of motion for the orientation vector are non-singular.

2.15 Projects

Exercise 2.18: Free Rigid Body

Write and demonstrate a program that reproduces diagrams like figure 2.3. Can you find trajectories that are asymptotic to the unstable relative equilibrium on the intermediate principal axis?

Exercise 2.19: Rotation of Mercury

In the 60's it was discovered that Mercury has a rotation period that is precisely 2/3 times its orbital period. We can see this resonant behavior in the spin-orbit model problem, and we can also play with nudging Mercury a bit to see how far off the rotation rate can be and still be trapped in this spin-orbit resonance. If the mismatch in angular velocity is too great, Mercury's rotation is no longer resonantly locked to its orbit. Set $\epsilon = 0.026$ and $e = 0.2$.

a. Write a program for the spin-obit problem so this resonance dynamics can be investigated numerically. You will need to know (or, better, show!) that f satisfies the equation

$$Df = n(1-e^2)^{1/2}\left(\frac{a}{r}\right)^2, \tag{2.152}$$

with

$$\frac{a}{r} = \frac{1+e\cos f}{1-e^2}. \tag{2.153}$$

b. Show that the 3:2 resonance is stable by numerically integrating the system when the rotation is not exactly in resonance and observing that the angle $\theta - \frac{3}{2}f$ oscillates.

c. Find the range of initial $\dot{\theta}$ for which this resonance angle oscillates.

Exercise 2.20: Precession of the Equinox

The Earth spins very nearly about the largest moment of inertia, and the spin axis is tilted by about 23° to the orbit normal. There is a gravity-gradient torque on the Earth from the Sun that causes the spin-axis of the Earth to precess. Investigate this precession in the approximation that the orbit of the Earth is circular, and the Earth is axisymmetric. Determine the rate of precession in terms of the moments of inertia of the Earth.

3
Hamiltonian Mechanics

The formulation of mechanics with generalized coordinates and momenta as dynamical state variables is called the Hamiltonian formulation. The Hamiltonian formulation of mechanics is equivalent to the Lagrangian formulation, however each presents a useful point of view. The Lagrangian formulation is especially useful in the initial formulation of a system. The Hamiltonian formulation is especially useful in understanding the evolution, especially when there are symmetries and conserved quantities.

For each continuous symmetry of a mechanical system there is a conserved quantity. If the generalized coordinates can be chosen to reflect a symmetry, then, by the Lagrange equations, the conjugate momentum is conserved. We have seen that such conserved quantities allow us to deduce important properties of the motion. For instance, consideration of the energy and angular momentum allowed us to deduce that rotation of a free rigid body about the axis of intermediate moment of inertia is unstable, and that rotation about the other principal axes is stable. For the axisymmetric top, we used two conserved momenta to reexpress the equations governing the evolution of the tilt angle so that they only involve the tilt angle and its derivative. The evolution of the tilt angle can be determined independently and has simply periodic solutions. Consideration of the conserved momenta has provided key insight. The Hamiltonian formulation is motivated by the desire to focus attention on the momenta.

In the Lagrangian formulation the momenta are, in a sense, secondary quantities: the momenta are functions of the state space variables, but the evolution of the state space variables depends on the state space variables and not on the momenta. To make use of any conserved momenta requires fooling around with the specific equations. The momenta can be rewritten in terms of the coordinates and the velocities, so, locally, we can solve for the velocities in terms of the coordinates and momenta. For a given mechanical system and given coordinates, the momenta and the velocities can be deduced from one another. Thus we can represent the dynamical state of the system in terms of the coordinates and momenta just as well as with the coordinates and the velocities. If we use the coordinates and momenta to represent the state and write the associated state derivative in terms of the coordinates and momenta, then we have a self contained system. This formulation of the equations governing the evolution of the system has the advantage that if some of the momenta are conserved, the remaining equations are immediately simplified.

The Lagrangian formulation of mechanics has provided the means to investigate the motion of complicated mechanical systems. We have found that dynamical systems exhibit a bewildering variety of possible motions. The motion is sometimes rather simple, and sometimes the motion is very complicated. Sometimes the evolution depends very sensitively on the initial conditions, and sometimes it is insensitive. And sometimes there are orbits that maintain resonance relationships with a drive. Consider the periodically driven pendulum. The driven pendulum can behave more or less as an undriven pendulum with extra wiggles. It can move in a strongly chaotic manner. It can move in resonance with the drive, oscillating once for every two cycles of the drive, or looping around once per drive cycle. Or consider the Moon. The Moon rotates synchronously with its orbital motion, always pointing roughly the same face to the Earth. However, Mercury rotates three times every two times it circles the Sun, and Hyperion rotates chaotically. How can we make sense of this? How do we put the possible motions of these systems in relation to each other? What other motions are possible? The Hamiltonian formulation of dynamics gives us much more than the stated goal of expressing the system derivative in terms of potentially conserved quantities. The Hamiltonian formulation provides a convenient framework in which the possible motions may be placed and understood. We will be able to see the range of stable resonance motions, and the range of states reached by chaotic trajectories, and discover other unsuspected possible motions. The Hamiltonian formulation leads to many additional insights.

3.1 Hamilton's Equations

The momenta are given by momentum state functions of the time, the coordinates, and the velocities.[1] Locally we can find inverse functions that give the velocities in terms of the time, the coordinates, and the momenta. We can use this inverse function to represent the state in terms of the coordinates and momenta rather than the coordinates and velocities. The equations of motion when recast in terms of coordinates and momenta are called *Hamilton's canonical equations*.

We present three derivations of Hamilton's equations. The first derivation is guided by the strategy outlined above and uses nothing more complicated than implicit functions and the chain rule. The second derivation first abstracts a key part of the first derivation and then applies the more abstract machinery to derive Hamilton's equations. The third uses the action principle.

Lagrange's equations give us the time derivative of the momentum p on a path q

$$Dp(t) = \partial_1 L(t, q(t), Dq(t)), \tag{3.1}$$

where

$$p(t) = \partial_2 L(t, q(t), Dq(t)). \tag{3.2}$$

To eliminate Dq we need to solve equation (3.2) for Dq in terms of p.

Let $\mathcal{V}$ be the function that gives the velocities in terms of the time, coordinates, and momenta. Defining $\mathcal{V}$ is a problem of functional inverses. To prevent confusion we use names for the variables that do not have mnemonic significance. Let

$$a = \partial_2 L(b, c, d), \tag{3.3}$$

[1] Here we restrict our attention to Lagrangians that only depend on the time, the coordinates, and the velocities.

then $\mathcal{V}$ satisfies[2]

$$d = \mathcal{V}(b, c, a). \tag{3.4}$$

The Lagrange equation (3.1) can be rewritten in terms of p using $\mathcal{V}$:

$$Dp(t) = \partial_1 L(t, q(t), \mathcal{V}(t, q(t), p(t))). \tag{3.5}$$

We can also use $\mathcal{V}$ to rewrite equation (3.2) as an equation for Dq in terms of t, q and p:

$$Dq(t) = \mathcal{V}(t, q(t), p(t)). \tag{3.6}$$

Equations (3.5) and (3.6) give the rate of change of q and p along realizable paths as functions of t, q, and p along the paths.

Though fulfilling our goal of expressing the equations of motion entirely in terms of coordinates and momenta, we can find a more convenient representation. Define the function

$$\widetilde{L}(t, q, p) = L(t, q, \mathcal{V}(t, q, p)), \tag{3.7}$$

which is the Lagrangian reexpressed as a function of time, coordinates, and momenta. For the equations of motion we need $\partial_1 L$ evaluated with the appropriate arguments. Consider

$$\begin{aligned} \partial_1 \widetilde{L}(t, q, p) &= \partial_1 L(t, q, \mathcal{V}(t, q, p)) + \partial_2 L(t, q, \mathcal{V}(t, q, p)) \partial_1 \mathcal{V}(t, q, p) \\ &= \partial_1 L(t, q, \mathcal{V}(t, q, p)) + p \partial_1 \mathcal{V}(t, q, p), \end{aligned} \tag{3.8}$$

where we used the chain rule in the first step and the inverse property of $\mathcal{V}$ in the second step. Introducing the momentum selector $P(t, q, p) = p$, and using the property $\partial_1 P = 0$, we have

$$\begin{aligned} \partial_1 L(t, q, \mathcal{V}(t, q, p)) &= \partial_1 \widetilde{L}(t, q, p) - P(t, q, p) \partial_1 \mathcal{V}(t, q, p) \\ &= \partial_1 (\widetilde{L} - P\mathcal{V})(t, q, p) \\ &= -\partial_1 H(t, q, p), \end{aligned} \tag{3.9}$$

[2] The following properties hold:
$d = \mathcal{V}(b, c, \partial_2 L(b, c, d))$
$a = \partial_2 L(b, c, \mathcal{V}(b, c, a))$.

where the *Hamiltonian* H is defined by[3]

$$H = P\mathcal{V} - \widetilde{L}. \tag{3.10}$$

The Lagrange equation for Dp becomes simply

$$Dp(t) = -\partial_1 H(t, q(t), p(t)). \tag{3.11}$$

The equation for Dq can also be written in terms of H. Consider

$$\begin{aligned}\partial_2 H(t, q, p) &= \partial_2(P\mathcal{V} - \widetilde{L})(t, q, p) \\ &= \mathcal{V}(t, q, p) + p\partial_2\mathcal{V}(t, q, p) - \partial_2\widetilde{L}(t, q, p).\end{aligned} \tag{3.12}$$

To carry out the derivative of $\widetilde{L}$ we write it out in terms of L:

$$\partial_2\widetilde{L}(t, q, p) = \partial_2 L(t, q, \mathcal{V}(t, q, p))\partial_2\mathcal{V}(t, q, p) = p\partial_2\mathcal{V}(t, q, p), \tag{3.13}$$

using the inverse property of $\mathcal{V}$ again. So, putting equations (3.12) and (3.13) together, we obtain

$$\partial_2 H(t, q, p) = \mathcal{V}(t, q, p). \tag{3.14}$$

On paths for which $Dq(t) = \mathcal{V}(t, q(t), p(t))$ we have

$$Dq(t) = \partial_2 H(t, q(t), p(t)). \tag{3.15}$$

Equations (3.11) and (3.15) give the derivatives of the coordinate and momentum path functions in terms of the time, coordinates, and momenta. These equations are known as *Hamilton's equations*:[4]

$$\begin{aligned}Dq(t) &= \partial_2 H(t, q(t), p(t)) \\ Dp(t) &= -\partial_1 H(t, q(t), p(t)).\end{aligned} \tag{3.16}$$

---

[3] The overall minus sign in the definition of the Hamiltonian is traditional.

[4] In traditional notation Hamilton's equations are written:

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} \quad \text{and} \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q},$$

or as separate equations for each component:

$$\frac{dq^i}{dt} = \frac{\partial H}{\partial p_i} \quad \text{and} \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q^i}.$$

The first equation is just a restatement of the relationship of the momenta to the velocities in terms of the Hamiltonian and holds for any path, whether or not it is a realizable path. The second equation holds only for realizable paths.

Hamilton's equations have an especially simple and symmetrical form. Just as Lagrange's equations are constructed from a real-valued function, the Lagrangian, Hamilton's equations are constructed from a real-valued function, the Hamiltonian. The Hamiltonian function is[5]

$$H(t, q, p) = p\mathcal{V}(t, q, p) - L(t, q, \mathcal{V}(t, q, p)). \tag{3.17}$$

The Hamiltonian has the same value as the energy function $\mathcal{E}$ (see equation 1.122), except that the velocities are expressed in terms of time, coordinates, and momenta by $\mathcal{V}$:

$$H(t, q, p) = \mathcal{E}(t, q, \mathcal{V}(t, q, p)). \tag{3.18}$$

Illustration

Let's try something simple: the motion of a particle of mass m with potential energy $V(x, y)$. A Lagrangian is

$$L(t; x, y; v_x, v_y) = \tfrac{1}{2}m(v_x^2 + v_y^2) - V(x, y). \tag{3.19}$$

To form the Hamiltonian we first find the momenta $p = \partial_2 L(t, q, v)$: $p_x = mv_x$ and $p_y = mv_y$. Solving for the velocities in terms of the momenta is easy here: $v_x = p_x/m$ and $v_y = p_y/m$. The Hamiltonian is $H(t, q, p) = pv - L(t, q, v)$ with v reexpressed in terms of (t, q, p):

$$H(t; x, y; p_x, p_y) = \frac{p_x^2 + p_y^2}{2m} + V(x, y). \tag{3.20}$$

The kinetic energy is a homogeneous quadratic form in the velocities, so the energy is $T + V$ and the Hamiltonian is the energy expressed in terms of momenta rather than velocities. Hamilton's

[5]Traditionally, the Hamiltonian is written

$$H = p\dot{q} - L,$$

This way of writing the Hamiltonian confuses the values of functions with the functions that generate them: both $\dot{q}$ and L have to be reexpressed as functions of the time, coordinates and momenta.

equations for Dq are

$$Dx = p_x/m$$
$$Dy = p_y/m. \tag{3.21}$$

Note that on paths, where $v_x = Dx$ and $v_y = Dy$, these just restate the relation between the momenta and the velocities. Hamilton's equations for Dp are

$$Dp_x = -\partial_0 V(x, y)$$
$$Dp_y = -\partial_1 V(x, y). \tag{3.22}$$

The rate of change of the linear momentum is minus the gradient of the potential energy.

Exercise 3.1: Deriving Hamilton's Equations

For each of the following Lagrangians derive the Hamiltonian and Hamilton's equations. These problems are simple enough to do by hand.

a. A Lagrangian for a planar pendulum is $L(t, \theta, \dot{\theta}) = \frac{1}{2}ml^2\dot{\theta}^2 + mgl\cos\theta$.

b. A Lagrangian for a particle of mass m with a two dimensional potential energy $V(x, y) = (x^2 + y^2)/2 + x^2y - y^3/3$ is $L(t; x, y; \dot{x}, \dot{y}) = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) - V(x, y)$.

c. A Lagrangian for a particle of mass m constrained to move on a sphere of radius R is $L(t; \theta, \varphi; \dot{\theta}, \dot{\varphi}) = \frac{1}{2}mR^2(\dot{\theta}^2 + (\dot{\varphi}\sin\theta)^2)$, where θ is the colatitude and φ is the longitude on the sphere.

Exercise 3.2: Sliding Pendulum

For the pendulum with a sliding support (see Exercise 1.22) derive a Hamiltonian and Hamilton's equations.

Hamiltonian State

Given a coordinate path q, and a Lagrangian L, the corresponding momentum path p is given by equation (3.2). Equation (3.15) expresses the same relationship in terms of the corresponding Hamiltonian H. That these relations are valid for any path, whether or not it is a realizable path, allows us to abstract to arbitrary velocity and momentum at a moment. At a moment, the momentum p for the state tuple (t, q, v) is $p = \partial_2 L(t, q, v)$. We also have $v = \partial_2 H(t, q, p)$. In the Lagrangian formulation the state of the system at a moment can be specified by the local state tuple (t, q, v) of time, generalized coordinates, and generalized velocities. Lagrange's equations determine a unique path emanating from this state. In the Hamiltonian formulation the state can be specified by the tuple (t, q, p) of time, generalized coordinates, and generalized momenta. Hamilton's equations determine a unique path emanating from this state. The Lagrangian state tuple (t, q, v) encodes exactly the same information as the Hamiltonian state tuple (t, q, p); we need a Lagrangian or a Hamiltonian to relate them. The two formulations are equivalent in that for equivalent initial states the same coordinate path emanates from them.

The Lagrangian state derivative is constructed from the Lagrange equations by solving for the highest order derivative and abstracting to arbitrary positions and velocities at a moment.[6] The Lagrangian state path is generated by integration of the Lagrangian state derivative given an initial Lagrangian state (t, q, v). Similarly, the Hamiltonian state derivative can be constructed from Hamilton's equations by abstracting to arbitrary positions and momenta at a moment. Hamilton's equations are a set of first-order differential equations in explicit form. The Hamiltonian state derivative can be directly written in terms of them. The Hamiltonian state path is generated by integration of the Hamiltonian state derivative given an initial Hamiltonian state (t, q, p). If these state paths are obtained by integrating the state derivatives with equivalent initial states, then the coordinate path component of these state paths are the same and satisfy the Lagrange equations. The coordinate path and the momentum path components of the Hamiltonian state path satisfy Hamilton's equations. The Hamiltonian formulation and the Lagrangian formulation are equivalent.

Given a path q the Lagrangian state path and the Hamiltonian state paths can be deduced from it. The Lagrangian state path $\Gamma[q]$ can be constructed from a path q simply by taking derivatives. The Lagrangian state path satisfies:

$$\Gamma[q](t) = (t, q(t), Dq(t)) . \tag{3.23}$$

[6] In the construction of the Lagrangian state derivative from the Lagrange equations we must solve for the highest order derivative. The solution process requires the inversion of the matrix $\partial_2\partial_2 L$. In the construction of Hamilton's equations, the construction of $\mathcal{V}$ from the momentum state function $\partial_2 L$ requires the inversion of the same matrix. If the Lagrangian formulation has singularities, the singularities cannot be avoided by going to the Hamiltonian formulation.

The Lagrangian state path is uniquely determined by the path q. The Hamiltonian state path $\Pi_L[q]$ can also be constructed from the path q but the construction requires a Lagrangian. The Hamiltonian state path satisfies

$$\Pi_L[q](t) = (t, q(t), \partial_2 L(t, q(t), Dq(t))) = (t, q(t), p(t)) . \tag{3.24}$$

The Hamiltonian state tuple is not uniquely determined by the path q because it depends upon our choice of Lagrangian, which is not unique.

The $2n$-dimensional space whose elements are labeled by the n generalized coordinates q^i and the n generalized momenta p_i is called *phase space*. The components of the generalized coordinates and momenta are collectively called the *phase-space components*.[7] The dynamical state of the system is completely specified by the phase state tuple (t, q, p), given a Lagrangian or Hamiltonian to provide the map between velocities and momenta.

Computing Hamilton's Equations

Hamilton's equations are a system of first order differential equations. We presented a procedural formulation of Lagrange's equations as a first order system in section 1.8. The following formulation of Hamilton's equations is analogous:

```
(define ((Hamilton-equations Hamiltonian) q p)
  (let ((H-state-path (qp->H-state-path q p)))
    (- (D H-state-path)
       (compose (phase-space-derivative Hamiltonian)
                H-state-path))))
```

The Hamiltonian state derivative is computed as follows:

---

[7]The term *phase space* was introduced by Josiah Willard Gibbs in his formulation of statistical mechanics. The Hamiltonian plays a fundamental role in the Boltzmann-Gibbs formulation of statistical mechanics, and in both the Heisenberg and Schrödinger approaches to quantum mechanics.

The momentum p can be viewed as the coordinate representation of a linear form on the tangent space. Thus $p\dot{q}$ is a scalar quantity, which is invariant under time-independent coordinate transformations of the configuration space. The set of momentum forms comprise an n-dimensional vector space at each point of configuration space called the *cotangent space*. The collection of all cotangent spaces of a configuration space forms a space called the *cotangent bundle* of the configuration manifold.

```
(define ((phase-space-derivative Hamiltonian) H-state)
  (->H-state 1
             (((partial 2) Hamiltonian) H-state)
             (- (((partial 1) Hamiltonian) H-state))))
```

The state in the Hamiltonian formulation is composed of the time, the coordinates, and the momenta. We call this an `H-state`, to distinguish it from the state in the Lagrangian formulation. We can select the components of the Hamiltonian state with the selectors `time`, `coordinate`, `momentum`. We construct Hamiltonian states from their components with `->H-state`. The first component of the state is time, so the first component of the state derivative is one, the time rate of change of time. Given procedures `q` and `p` implementing coordinate and momentum path functions, the Hamiltonian state path can be constructed with the following procedure:

```
(define ((qp->H-state-path q p) t)
  (->H-state t (q t) (p t)))
```

The `Hamilton-equations` procedure returns the residuals of Hamilton's equations for the given paths.

For example, a procedure implementing the Hamiltonian for a point mass with potential energy $V(x, y)$ is

```
(define ((H-rectangular m V) H-state)
  (let ((q (coordinate H-state))
        (p (momentum H-state)))
    (+ (/ (square p) (* 2 m))
       (V (ref q 0) (ref q 1)))))
```

Hamilton's equations are:[8]

[8] By default literal functions map reals to reals; the default type for a literal function is `(-> Real Real)`. Here, the potential energy `V` takes two real arguments and returns a real.

```
(show-expression
 (((Hamilton-equations
     (H-rectangular
         'm
         (literal-function 'V (-> (X Real Real) Real))))
    (coordinate-tuple (literal-function 'x)
                      (literal-function 'y))
    (momentum-tuple (literal-function 'p_x)
                    (literal-function 'p_y)))
   't))
```

$$\begin{pmatrix} 0 \\ \begin{pmatrix} Dx\,(t) - \dfrac{p_x\,(t)}{m} \\ Dy\,(t) - \dfrac{p_y\,(t)}{m} \end{pmatrix} \\ \begin{bmatrix} Dp_x\,(t) + \partial_0 V\,(x\,(t)\,, y\,(t)) \\ Dp_y\,(t) + \partial_1 V\,(x\,(t)\,, y\,(t)) \end{bmatrix} \end{pmatrix}$$

The zero in first element of the structure of Hamilton's equations residuals is just the tautology that time advances uniformly: that the time function is just the identity, so its derivative is 1 and the residual is zero. The equations in the second element relates the coordinate paths and the momentum paths. The equations in the third element give the rate of change of the momenta in terms of the applied forces.

Exercise 3.3: Computing Hamilton's Equations

Check your answers to Exercise 3.1 with the Hamilton equations procedures.

3.1.1 The Legendre transformation

The Legendre transformation abstracts a key part of the process of transforming from the Lagrangian to the Hamiltonian formulation of mechanics — the replacement of functional dependence on generalized velocities with functional dependence on generalized momenta. The momentum state function is defined as a partial derivative of the Lagrangian, a real-valued function of time, coordinates, and velocities. The Legendre transformation provides an inverse that gives the velocities in terms of the momenta: we are able to write the velocities as a partial derivative of a different real-valued function of time, coordinates, and momenta.[9]

Given a real-valued function F, if we can find a real-valued function G, such that $DF = (DG)^{-1}$ then we say that F and G are related by a Legendre transform.

Locally we can define the inverse function[10] $\mathcal{V}$ of DF so that $DF \circ \mathcal{V} = I$, where I is the identity function $I(w) = w$. Consider the composite function $\widetilde{F} = F \circ \mathcal{V}$. The derivative of $\widetilde{F}$ is

$$D\widetilde{F} = (DF \circ \mathcal{V})D\mathcal{V} = ID\mathcal{V}. \tag{3.25}$$

Using the product rule and $DI = 1$,

$$D\widetilde{F} = D(I\mathcal{V}) - \mathcal{V}, \tag{3.26}$$

or

$$\mathcal{V} = D(I\mathcal{V}) - D\widetilde{F} = D(I\mathcal{V} - \widetilde{F}). \tag{3.27}$$

The integral is determined up to a constant of integration. If we define

$$G = I\mathcal{V} - \widetilde{F}, \tag{3.28}$$

then we have

$$\mathcal{V} = DG. \tag{3.29}$$

The function G has the desired property that DG is the inverse function $\mathcal{V}$ of DF. The derivation just given applies equally well if the arguments of F and G have multiple components.

Given a relation $w = DF(v)$ for some given function F, then $v = DG(w)$ for $G = I\mathcal{V} - F \circ \mathcal{V}$, where $\mathcal{V}$ is the inverse function of DF provided it exists.

A picture may help (see Figure 3.1). The curve is the graph of the function DF. Turned sideways, it is also the graph of the function DG, because DG is the inverse function of DF. The integral of DF from v_0 to v is $F(v) - F(v_0)$; this is the area below

[9]The Legendre transformation is more general than its use in mechanics in that it captures the relationship between conjugate variables in systems as diverse as thermodynamics, circuits, and field theory.

[10]This can be done so long as the derivative is not zero.

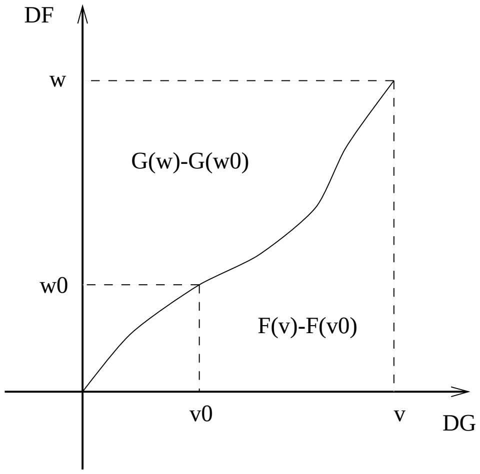

Figure 3.1 The Legendre transform can be interpreted in terms of geometric areas. The curve is the graph of DF, and viewed sideways is the graph of $DG = DF^{-1}$. This figure should remind you of the geometric interpretation of the product rule for derivatives, or alternatively, integration by parts.

the curve from v_0 to v. Likewise the integral of DG from w_0 to w is $G(w) - G(w_0)$; this is the area to the left of the curve from w_0 to w. The union of these two regions has the area $wv - w_0 v_0$. So

$$wv - w_0 v_0 = F(v) - F(v_0) + G(w) - G(w_0), \tag{3.30}$$

which is the same as

$$wv - F(v) - G(w) = w_0 v_0 - G(w_0) - F(v_0). \tag{3.31}$$

The left-hand side depends on the point labeled by w and v and the right-hand side depends on the point labeled by w_0 and v_0, so these can only be equal to a constant, independent of the variable endpoints. As the point is changed the combination $G(w)+F(v)-wv$ is invariant. So

$$G(w) = wv - F(v) + C, \tag{3.32}$$

with constant C. The requirement for G depends only on DG so we can choose to define G with $C = 0$.

Legendre transformations with passive arguments

Let F be a real-valued function of two arguments, and

$$w = \partial_1 F(x, v). \tag{3.33}$$

If we can find a real-valued function G such that

$$v = \partial_1 G(x, w) \tag{3.34}$$

we say that F and G are related by a Legendre transformation, and that the second argument in each function is *active* and that the first argument is *passive* in the transformation.

If the function $\partial_1 F$ can be locally inverted with respect to the second argument we can define

$$v = \mathcal{V}(x, w), \tag{3.35}$$

giving

$$w = \partial_1 F(x, \mathcal{V}(x, w)) = W(x, w), \tag{3.36}$$

where W is the selector function for the second argument.

For the active arguments the derivation goes through as before. The first argument to F and G is just along for the ride, it is a passive argument. Let

$$\widetilde{F}(x, w) = F(x, \mathcal{V}(x, w)), \tag{3.37}$$

then define

$$G = W\mathcal{V} - \widetilde{F}. \tag{3.38}$$

We can check that G has the property $\mathcal{V} = \partial_1 G$ by carrying out the derivative:

$$\begin{aligned}\partial_1 G &= \partial_1(W\mathcal{V} - \widetilde{F}) \\ &= \mathcal{V} + W\partial_1\mathcal{V} - \partial_1\widetilde{F},\end{aligned} \tag{3.39}$$

but

$$\begin{aligned}\partial_1\widetilde{F}(x, w) &= \partial_1 F(x, \mathcal{V}(x, w))\partial_1\mathcal{V}(x, w) \\ &= W(x, w)\partial_1\mathcal{V}(x, w),\end{aligned} \tag{3.40}$$

or

$$\partial_1 \widetilde{F} = W \partial_1 \mathcal{V}. \tag{3.41}$$

So

$$\partial_1 G = \mathcal{V}, \tag{3.42}$$

as required. The active argument may have many components.

The partial derivatives with respect to the passive arguments are related in a remarkably simple way. Let's calculate the derivative $\partial_0 G$ in pieces. First,

$$\partial_0 (W \mathcal{V}) = W \partial_0 \mathcal{V} \tag{3.43}$$

because $\partial_0 W = 0$. To calculate $\partial_0 \widetilde{F}$ we must supply arguments

$$\begin{aligned}\partial_0 \widetilde{F}(x, w) &= \partial_0 F(x, \mathcal{V}(x, w)) + \partial_1 F(x, \mathcal{V}(x, w)) \partial_0 \mathcal{V}(x, w) \\ &= \partial_0 F(x, \mathcal{V}(x, w)) + W(x, w) \partial_0 \mathcal{V}(x, w).\end{aligned} \tag{3.44}$$

Putting these together we find

$$\partial_0 G(x, w) = -\partial_0 F(x, \mathcal{V}(x, w)) = -\partial_0 F(x, v). \tag{3.45}$$

The calculation is unchanged if the passive argument has many components.

We can write the Legendre transformation more symmetrically:

$$\begin{aligned} w &= \partial_1 F(x, v) \\ wv &= F(x, v) + G(x, w) \\ v &= \partial_1 G(x, w) \\ 0 &= \partial_0 F(x, v) + \partial_0 G(x, w). \end{aligned} \tag{3.46}$$

The last relation is not as trivial as it looks, because x enters the equations connecting w and v. With this symmetrical form, we see that the Legendre transform is its own inverse.

Exercise 3.4: Simple Legendre transforms

For each of the following functions find the function that is related to the given function by the Legendre transform on the indicated active argument. Show that the Legendre transform relations hold for your solution, including the relations among passive arguments, if any.

a. $F(x) = a \sin x + b \cos x$, there are no passive arguments.

b. $F(x, y) = a \sin x \cos y$, with x active.

c. $F(x, y, \dot{x}, \dot{y}) = x\dot{x}^2 + 3\dot{x}\dot{y} + y\dot{y}^2$, with $\dot{x}$ and $\dot{y}$ active.

Hamilton's Equations from the Legendre Transformation

We can use the Legendre transformation with the Lagrangian playing the role of F and with the generalized velocity slot playing the role of the active argument. The Hamiltonian plays the role of G with the momentum slot active. The coordinate and time slots are passive arguments.

The Lagrangian L and the Hamiltonian H are related by a Legendre transformation:

$$e = (\partial_2 L)(a, b, c) \tag{3.47}$$

$$ec = L(a, b, c) + H(a, b, e) \tag{3.48}$$

and

$$c = (\partial_2 H)(a, b, e), \tag{3.49}$$

with passive equations

$$0 = \partial_0 L(a, b, c) + \partial_0 H(a, b, e), \tag{3.50}$$
$$0 = \partial_1 L(a, b, c) + \partial_1 H(a, b, e). \tag{3.51}$$

Presuming it exists, we can define the inverse of $\partial_2 L$ with respect to the last argument

$$c = \mathcal{V}(a, b, e). \tag{3.52}$$

and write the Hamiltonian

$$H(a, b, c) = c\mathcal{V}(a, b, c) - L(a, b, \mathcal{V}(a, b, c)). \tag{3.53}$$

These relations are purely algebraic in nature.

On a path q we have the momentum p:

$$p(t) = \partial_2 L(t, q(t), Dq(t)), \tag{3.54}$$

and from the definition of $\mathcal{V}$

$$Dq(t) = \mathcal{V}(t, q(t), p(t)). \tag{3.55}$$

The Legendre transform gives

$$Dq(t) = \partial_2 H(t, q(t), p(t)). \tag{3.56}$$

This relation is purely algebraic and is valid for any path. The passive equation (3.51) gives

$$\partial_1 L(t, q(t), Dq(t)) = -\partial_1 H(t, q(t), p(t)), \tag{3.57}$$

but the left-hand side can be rewritten using the Lagrange equations, so

$$Dp(t) = -\partial_1 H(t, q(t), p(t)). \tag{3.58}$$

This equation is only valid for realizable paths, because we used the Lagrange equations to derive it. Equations (3.56) and (3.58) are Hamilton's equations.

The remaining passive equation is

$$\partial_0 L(t, q(t), Dq(t)) = -\partial_0 H(t, q(t), p(t)). \tag{3.59}$$

We have found that if the Lagrangian has no explicit time dependence ($\partial_0 L = 0$) then energy is conserved. This passive equation says that if the Lagrangian has no explicit time dependence then the Hamiltonian will also have no explicit time dependence ($\partial_0 H = 0$). So if the Hamiltonian has no explicit time dependence then it is a conserved quantity.

Exercise 3.5:

Using Hamilton's equations, show directly that the Hamiltonian is a conserved quantity if the Hamiltonian has no explicit time dependence.

Legendre Transforms of Quadratic Functions

We cannot implement the Legendre transform in general because it involves finding the functional inverse of an arbitrary function. However, many physical systems can be described by Lagrangians that are quadratic forms in the generalized velocities. For such functions the generalized momenta are linear functions of the generalized velocities, and thus explicitly invertible.

More generally, we can compute a Legendre transformation for polynomial functions where the leading term is a quadratic form:

$$F(v) = \frac{1}{2}vMv + bv + c. \tag{3.60}$$

We can assume M is symmetric,[11] because it defines a quadratic form. We can find linear expressions for w

$$w = DF(v) = vM + b. \tag{3.61}$$

So if M is invertible we can solve for v in terms of w. Thus we may define a function $\mathcal{V}$ such that

$$v = \mathcal{V}(w) = M^{-1}(w - b) \tag{3.62}$$

and we can use this to compute the value of the function G:

$$G(w) = w\mathcal{V}(w) - F(\mathcal{V}(w)). \tag{3.63}$$

Computing Hamiltonians

We implement the Legendre transform for quadratic functions by the procedure:[12]

```
(define (Legendre-transform F)
  (let ((w-of-v (D F)))
    (define (G w)
      (let ((z (dual-zero w)))
        (let ((M ((D w-of-v) z))
              (b (w-of-v z)))
          (let ((v (/ (- w b) M)))
            (- (* w v) (F v))))))
    G))
```

The procedure `Legendre-transform` takes a procedure of one argument and returns the procedure that is associated with it by the Legendre transform. If $w = DF(v)$, $wv = F(v) + G(w)$, and $v = DG(w)$ specifies a one argument Legendre transformation,

---

[11] Let $\mathbf{M}$ be the matrix representation of M, then $\mathbf{M} = \mathbf{M}^{\mathsf{T}}$.

[12] The division operation, denoted by `/` in the `Legendre-transform` procedure, is generic over mathematical objects. We interpret the division in the matrix representation: if a vector $\mathbf{y}$ is divided by a matrix $\mathbf{M}$ this is interpreted as a request to solve the linear system $\mathbf{Mx} = \mathbf{y}$, where $\mathbf{x}$ is the unknown vector.

then G is the function associated with F by the Legendre transform: $G = I\mathcal{V} - F \circ \mathcal{V}$, where $\mathcal{V}$ is the functional inverse of DF.

We can use the `Legendre-transform` procedure to compute a Hamiltonian from a Lagrangian

```
(define ((Lagrangian->Hamiltonian Lagrangian) H-state)
  (let ((t (time H-state))
        (q (coordinate H-state))
        (p (momentum H-state)))
    (define (L qdot)
      (Lagrangian (->local t q qdot)))
    ((Legendre-transform L) p)))
```

Notice that the one-argument `Legendre-transform` procedure is sufficient. The passive variables are given no special attention, they are just passed around.

The Lagrangian may be obtained from the Hamiltonian by the procedure:

```
(define ((Hamiltonian->Lagrangian Hamiltonian) L-state)
  (let ((t (time L-state))
        (q (coordinate L-state))
        (qdot (velocity L-state)))
    (define (H p)
      (Hamiltonian (->H-state t q p)))
    ((Legendre-transform H) qdot)))
```

Notice that the two procedures `Hamiltonian->Lagrangian` and `Lagrangian->Hamiltonian` are identical, except for the names.

For example, the Hamiltonian for the motion of the point mass with the potential energy $V(x, y)$ may be computed from the Lagrangian:

```
(define ((L-rectangular m V) local)
  (let ((q (coordinate local))
        (qdot (velocity local)))
    (- (* 1/2 m (square qdot))
       (V (ref q 0) (ref q 1)))))
```

And the Hamiltonian is:

```
(show-expression
 ((Lagrangian->Hamiltonian
   (L-rectangular
      'm
      (literal-function 'V (-> (X Real Real) Real))))
  (->H-state 't
             (coordinate-tuple 'x 'y)
             (momentum-tuple 'p_x 'p_y))))
```

$$\boxed{V(x, y) + \frac{\frac{1}{2}p_x^2}{m} + \frac{\frac{1}{2}p_y^2}{m}}$$

Exercise 3.6: On a Helical Track

A uniform cylinder of mass M, radius R, and height h is mounted so as to rotate freely on a vertical axis. A mass point of mass m is constrained to move on a uniform frictionless helical track of pitch β (measured in radians per meter of drop along the cylinder) mounted on the surface of the cylinder (see figure 3.2). The mass is acted upon by standard gravity ($g = 9.8\text{ms}^{-2}$).

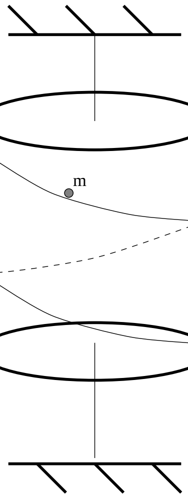

Figure 3.2

a. What are the degrees of freedom of this system? Pick and describe a convenient set of generalized coordinates for this problem. Write a Lagrangian to describe the dynamical behavior. It may help to know that the moment of inertia of the cylinder around its axis is $\frac{1}{2}MR^2$. You may find it easier to do the algebra if various constants are combined and represented as single symbols.

b. Make a Hamiltonian for the system. Write Hamilton's equations for the system. Are there any conserved quantities?

c. If we release the mass point at time $t = 0$ at the top of the track with zero initial speed and let it slide down, what is the motion of the system?

Exercise 3.7: An Ellipsoidal Bowl

Consider a point particle of mass m constrained to move in a bowl and acted upon by a uniform gravitational acceleration g. The bowl is ellipsoidal, with height $z = ax^2 + by^2$. Make a Hamiltonian for this system. Are there any immediate deductions you can make about this system?

3.1.2 Hamiltonian Action Principle

The previous two derivations of Hamilton's equations have made use of the Lagrange equations. Hamilton's equations can also be derived directly from the action principle.

The action is the integral of the Lagrangian along a path:

$$S[q](t_1, t_2) = \int_{t_1}^{t_2} L \circ \Gamma[q]. \tag{3.64}$$

The action is stationary with respect to variations of the path that preserve the configuration at the endpoints (for Lagrangians that are functions of time, coordinates, and velocities).

We can rewrite the integrand in terms of the Hamiltonian

$$L \circ \Gamma[q](t) = p(t)Dq(t) - H(t, q(t), p(t)), \tag{3.65}$$

with $p(t) = \partial_2 L(t, q(t), Dq(t))$. The Legendre transformation construction gives

$$Dq(t) = \partial_2 H(t, q(t), p(t)), \tag{3.66}$$

which is one of Hamilton's equations, the one that does not depend on the path being a realizable path. Using

$$\Pi_L[q](t) = (t, q(t), \partial_2 L(t, q(t), Dq(t))) = (t, q(t), p(t)), \tag{3.67}$$

the integrand is

$$L \circ \Gamma[q] = pDq - H \circ \Pi_L[q]. \tag{3.68}$$

The variation of the action is then

$$\begin{aligned}
\delta S[q](t_1, t_2) \\
&= \int_{t_1}^{t_2} \delta(pDq - H \circ \Pi_L[q]) \\
&= \int_{t_1}^{t_2} (\delta p \; Dq + p \; \delta Dq - (DH \circ \Pi_L[q]) \delta \Pi_L[q]) \\
&= \int_{t_1}^{t_2} \{\delta p \; Dq + p \; D\delta q \\
&\qquad - (\partial_1 H \circ \Pi_L[q])\delta q - (\partial_2 H \circ \Pi_L[q])\delta p\} ,
\end{aligned} \tag{3.69}$$

where δp is the variation in the momentum.[13] Integrating the second term by parts, using $D(p\delta q) = Dp\delta q + pD\delta q$, we get

$$\begin{aligned}
\delta S[q](t_1, t_2) &= p\delta q|_{t_1}^{t_2} \\
&+ \int_{t_1}^{t_2} \{\delta p \; Dq - Dp \; \delta q \\
&\qquad - (\partial_1 H \circ \Pi_L[q])\delta q - (\partial_2 H \circ \Pi_L[q])\delta p\} .
\end{aligned} \tag{3.70}$$

The variations are constrained so that $\delta q(t_1) = \delta q(t_2) = 0$ so the integrated part vanishes, so the variation of the action isan

$$\begin{aligned}
&\delta S[q](t_1, t_2) \\
&\quad = \int_{t_1}^{t_2} ((Dq - \partial_2 H \circ \Pi_L[q]) \, \delta p - (Dp + \partial_1 H \circ \Pi_L[q]) \, \delta q) .
\end{aligned} \tag{3.71}$$

---

[13] The variation of the momentum δp does not need to be further expanded in this argument because it turns out that the factor multiplying it is zero. However, it is handy to see how it is related to the variations in the coordinate path δq:

$$\delta p(t) = \partial_1 \partial_2 L(t, q(t), Dq(t))\delta q(t) + \partial_2 \partial_2 L(t, q(t), Dq(t)) D\delta q(t).$$

As a consequence of equation (3.66), the factor multiplying δp is zero. We are left with

$$\delta S[q](t_1, t_2) = \int_{t_1}^{t_2} (Dp + \partial_1 H \circ \Pi_L[q])\, \delta q. \tag{3.72}$$

For the variation of the action to be zero for arbitrary variations, except for the endpoint conditions, we must have

$$Dp = -\partial_1 H \circ \Pi_L[q], \tag{3.73}$$

which is the "dynamical" Hamilton's equation.[14]

3.1.3 A Wiring Diagram

Figure 3.3 shows a summary of the functional relationship between the Lagrangian and the Hamiltonian descriptions of a dynamical system. The diagram shows a "circuit" interconnecting some "devices" with "wires". The devices represent the mathematical functions that relate the quantities on their terminals. The wires represent identifications of the quantities on the terminals that they connect. For example, the box labeled L represents the Lagrangian function. Given values t, q, and $\dot{q}$ the value of the Lagrangian $L(t, q, \dot{q})$ is on the output o, which is wired to an input a_1 of an adder.

If one knows some of the pieces of the diagram, then other parts of the diagram can be computed. For instance, if we know the Lagrangian function, we can compute the derivative of the Lagrangian function, thus making the DL box explicit. If we further know the values of q and $\dot{q}$ at a time t, we can derive the output of the Lagrangian, and all the outputs $\partial L/\partial t$, $\partial L/\partial q$ and $\partial L/\partial \dot{q}$ of DL. This gives the value on the p wire and the $\dot{p}$ wire. The p and the $\dot{q}$ values give the output of the multiplier, which combined with the output of the Lagrangian (using the adder) gives the output of the Hamiltonian device.

---

[14] It is sometimes asserted that the momenta have a different status in the Lagrangian and Hamiltonian formulations; that in the Hamiltonian framework the momenta are "independent" of the coordinates. From this it is argued that the variations δq and δp are arbitrary and independent, therefore implying that the factor multiplying each of them in the action integral (3.72) must independently be zero, apparently deriving both of Hamilton's equations. The argument is fallacious: we can write δp in terms of δq (see footnote 13).

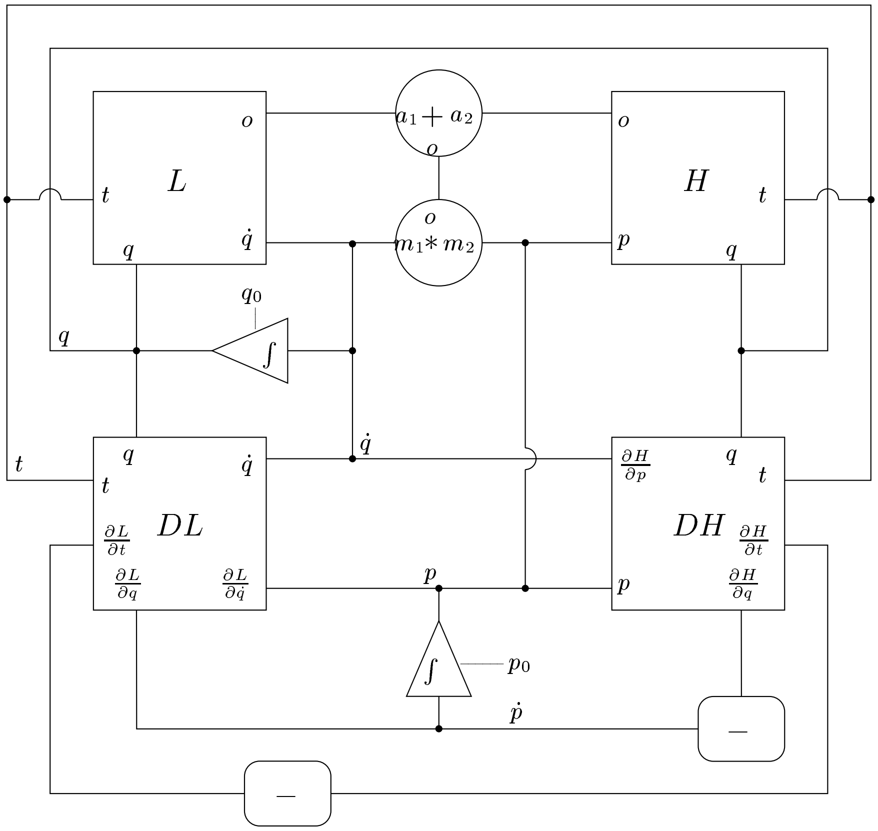

Figure 3.3 This is a "wiring diagram" describing the relationships among the dynamical quantities occurring in Lagrangian and Hamiltonian mechanics. A box, such as the one labeled L, represents a functional relation (the Lagrangian) among the quantities connected to its labeled terminals. For example, the sum of the outputs o of the Lagrangian and Hamiltonian is the product of the value on the $\dot{q}$ terminal of the Lagrangian and the value on the p terminal of the Hamiltonian. This fragment of the diagram summarizes the relationship of the Hamiltonian to the Lagrangian. The equations of motion are indicated by the presence of the integrators relating the dynamical quantities to their time derivatives.

One can use this diagram to plan a computation, and one can use it to understand the underlying unity of the Lagrangian and Hamiltonian formulations of mechanics. The active part of the Legendre transformation is represented by circuitry involving the adder and the multiplier. The connections made through the negation devices at the bottom of the diagram represent the passive part of the Legendre transformation. We see the second-order nature of mechanics by the fact that there are exactly two integrators, one relating the positions and the velocities and the other relating the momenta and their rates of change. Lagrange's equations are just the connection of the $\dot{p}$ wire to the $\partial L/\partial q$ terminal of the DL device. One of Hamilton's equations is just the connection of the $\dot{p}$ wire (through the negation device) to the $\partial H/\partial q$ terminal of the DH device. The other is just the connection of the $\dot{q}$ wire to the $\partial H/\partial p$ terminal of the DH device. We see that the two formulations are consistent. One does not have to abandon any part of the Lagrangian formulation to use the Hamiltonian formulation: there are deductions that can be made using both simultaneously.

3.2 Poisson Brackets

Here we introduce the *Poisson bracket*. In terms of the Poisson bracket Hamilton's equations have an elegant and symmetric expression.

Consider a function F of time, coordinates, and momenta. The value of F along the path $\sigma(t) = (t, q(t), p(t))$ is $(F \circ \sigma)(t) = F(t, q(t), p(t))$. The time derivative of $F \circ \sigma$ is

$$\begin{aligned} D(F \circ \sigma) &= (DF \circ \sigma) D\sigma \\ &= \partial_0 F \circ \sigma + (\partial_1 F \circ \sigma) Dq + (\partial_2 F \circ \sigma) Dp. \end{aligned} \tag{3.74}$$

If the phase-space path is a realizable path for a system with Hamiltonian H, then Dq and Dp can be reexpressed using Hamilton's equations

$$\begin{aligned} D(F \circ \sigma) &= \partial_0 F \circ \sigma + (\partial_1 F \circ \sigma)(\partial_2 H \circ \sigma) - (\partial_2 F \circ \sigma)(\partial_1 H \circ \sigma) \\ &= \partial_0 F \circ \sigma + (\partial_1 F \partial_2 H - \partial_2 F \partial_1 H) \circ \sigma \\ &= \partial_0 F \circ \sigma + \{F, H\} \circ \sigma \end{aligned} \tag{3.75}$$

where the Poisson bracket $\{F, H\}$ of F and H is defined by[15]

$$\{F, H\} = \partial_1 F \partial_2 H - \partial_2 F \partial_1 H. \tag{3.76}$$

Note that the Poisson bracket of two functions on the phase state space is also a function on the phase state space.

The coordinate selector Q is an example of a function on phase state space: $Q(t, q, p) = q$. According to equation (3.75)

$$Dq = D(Q \circ \sigma) = \{Q, H\} \circ \sigma = \partial_2 H \circ \sigma, \tag{3.77}$$

but this is the same as Hamilton's equation

$$Dq(t) = \partial_2 H(t, q(t), p(t)). \tag{3.78}$$

Similarly, the momentum selector P is a function on phase state space: $P(t, q, p) = p$. We have

$$Dp = D(P \circ \sigma) = \{P, H\} \circ \sigma = -\partial_1 H \circ \sigma, \tag{3.79}$$

which is the same as the other Hamilton's equation

$$Dp(t) = -\partial_1 H(t, q(t), p(t)). \tag{3.80}$$

So the Poisson bracket provides a uniform way of writing Hamilton's equations:

$$\begin{aligned} D(Q \circ \sigma) &= \{Q, H\} \circ \sigma \\ D(P \circ \sigma) &= \{P, H\} \circ \sigma. \end{aligned} \tag{3.81}$$

The Poisson bracket of any function with itself is zero, so we recover the conservation of energy for a system that has no explicit time dependence:

$$DE = D(H \circ \sigma) = (\partial_0 H + \{H, H\}) \circ \sigma = \partial_0 H \circ \sigma. \tag{3.82}$$

Properties of the Poisson bracket

Let F, G, and H be functions of time, position, and momentum, and c is independent of position and momentum.

[15] In traditional notation the Poisson bracket is written

$$\{F, H\} = \sum_i \left(\frac{\partial F}{\partial q^i} \frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial H}{\partial q^i} \right).$$

The Poisson bracket is antisymmetric:

$$\{F, G\} = -\{G, F\}. \tag{3.83}$$

It is bilinear (linear in each argument):

$$\begin{aligned}
\{F, G + H\} &= \{F, G\} + \{F, H\} && (3.84)\\
\{F, cG\} &= c\{F, G\} && (3.85)\\
\{F + G, H\} &= \{F, H\} + \{G, H\} && (3.86)\\
\{cF, G\} &= c\{F, G\}. && (3.87)
\end{aligned}$$

The Poisson bracket satisfies Jacobi's identity:

$$0 = \{F, \{G, H\}\} + \{H, \{F, G\}\} + \{G, \{H, F\}\}, \tag{3.88}$$

where all but the last can be immediately verified from the definition. Jacobi's identity requires a little more effort to verify.

Poisson Brackets of Conserved Quantities

The Poisson bracket of conserved quantities is conserved. Let F and G be time independent functions on the phase state space: $\partial_0 F = \partial_0 G = 0$. If F and G are conserved by the evolution under H then

$$\begin{aligned}
0 &= D(F \circ \sigma) = \{F, H\} \circ \sigma\\
0 &= D(G \circ \sigma) = \{G, H\} \circ \sigma && (3.89)
\end{aligned}$$

So the Poisson brackets of F and G with H are zero: $\{F, H\} = \{G, H\} = 0$. The Jacobi identity then implies

$$\{\{F, G\}, H\} = 0, \tag{3.90}$$

and thus

$$D(\{F, G\} \circ \sigma = 0, \tag{3.91}$$

so $\{F, G\}$ is a conserved quantity. The Poisson bracket of two conserved quantities is also a conserved quantity.

3.3 One degree of freedom

The solutions of time-independent systems with one degree of freedom can be found by quadrature. Such systems conserve the Hamiltonian: the Hamiltonian has a constant value on each realizable trajectory. We can use this constraint to eliminate the momentum in favor of the coordinate. Thus Hamilton's equations reduce to a single equation $Dq = f(q)$. The solution q can be expressed as a definite integral.

A geometric view reveals more structure. Time-independent systems with one degree of freedom have a two-dimensional phase space. Energy is conserved, so all orbits are level curves of the Hamiltonian. The possible orbit types are restricted to curves that are contours of a real-valued function. The possible orbits are paths of constant altitude in the mountain range on the phase plane described by the Hamiltonian.

There are a small number of characteristic features that are possible. There are points that are stable equilibria of the dynamical system. These are the peaks and pits of the Hamiltonian mountain range. These equilibria are stable in the sense that neighboring trajectories on nearby contours stay close to the equilibrium point. There are orbits that trace simple closed curves on contours that surround a peak or pit, or perhaps several peaks. There are also trajectories that lie on contours that cross at a saddle point. The crossing point is an unstable equilibrium. It is unstable in the sense that neighboring trajectories leave the vicinity of the equilibrium point. Such contours that cross at saddle points are called *separatrices*, a contour that "separates" two regions of distinct behavior.[16]

At every point Hamilton's equations give a unique rate of evolution. Hamilton's equations direct the system to move perpendicular to the gradient of the Hamiltonian. At the peaks, pits, and saddle points, the gradient of the Hamiltonian is zero, so according to Hamilton's equations these are fixed points. At other points, the gradient of the Hamiltonian is non-zero, so according to Hamilton's equations the rate of evolution is non-zero. Trajectories evolve along the contours of the Hamiltonian. Trajectories on simple closed contours periodically trace the contour. At a saddle point contours cross. The gradient of the Hamiltonian is

[16] *Separatrices* is the plural of *separatrix*.

zero at the saddle point so a system started at the saddle point does not leave the saddle point. On the separatrix away from the saddle point the gradient of the Hamiltonian is not zero so trajectories evolve along the contour. Trajectories on the separatrix are asymptotic forward or backward in time to a saddle point. Going forward or backward in time such trajectories forever approach an unstable equilibrium but never reach it. If the phase space is bounded, asymptotic trajectories that lie on contours of a smooth Hamiltonian are always asymptotic to unstable equilibria at both ends (but may be different equilibria).

These orbit types are all illustrated by the prototypical phase plane of the pendulum (see Figure 3.4). The solutions lie on contours of the Hamiltonian. There are three regions of the phase plane; in each the motion is qualitatively different. In the central region the pendulum oscillates; above this there is a region in which the pendulum circulates in one direction; and below the oscillation region the pendulum circulates in the other direction. In the center of the oscillation region there is a stable equilibrium, at which the pendulum is hanging motionless. At the boundaries between these regions the pendulum is asymptotic to the unstable equilibrium, at which the pendulum is standing upright.[17] There are two asymptotic trajectories, corresponding to the two ways the equilibrium can be approached. Each of these is also asymptotic to the unstable fixed point going backward in time.

3.4 Phase Space Reduction

Our motivation for the development of Hamilton's equations was to focus attention on the quantities that are sometimes conserved — the momenta and the energy. In the Hamiltonian formulation the generalized configuration coordinates and the conjugate momenta comprise the state of the system at a given time. We know from the Lagrangian formulation that if the Lagrangian does not depend on some coordinate then the conjugate momentum is conserved. This is also true in the Hamiltonian formulation, but there is a distinct advantage to the Hamiltonian formulation. In the Lagrangian formulation the knowledge of the conserved momentum

[17]The pendulum has only one unstable equilibrium. Remember that the coordinate is an angle.

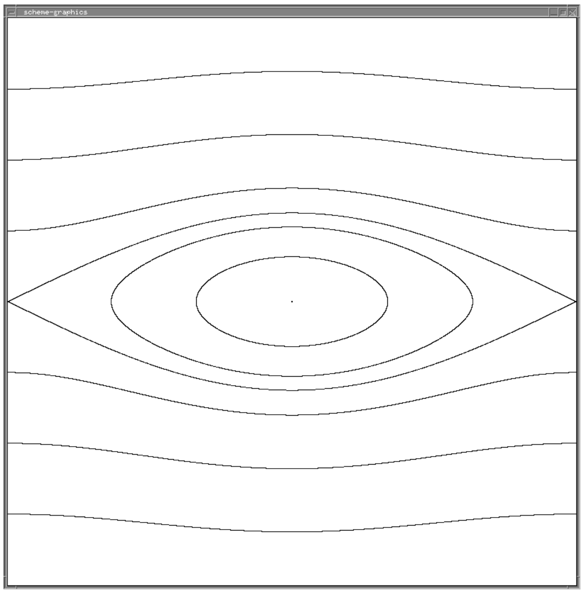

Figure 3.4 The phase plane of the pendulum has three regions displaying two distinct kinds of behavior. In this figure there are a number of different trajectories. Trajectories lie on the contours of the Hamiltonian. Trajectories may oscillate, making ovoid curves around the equilibrium point, or they may circulate, producing wavy tracks outside the eye-shaped region. The eye-shaped region is delimited by the separatrix. This pendulum has length 1m, a bob of mass 1kg, and the acceleration of gravity is $9.8\mathrm{ms}^{-2}$. The abscissa ranges from $-\pi$ to π, and the ordinate runs from $-20\mathrm{kgm}^2\mathrm{s}^{-1}$ to $20\mathrm{kgm}^2\mathrm{s}^{-1}$.

does not immediately lead to any simplification of the problem, but in the Hamiltonian formulation the fact that momenta are conserved gives an immediate reduction of the dimension of the system to be solved. In fact, if a coordinate does not appear in the Hamiltonian then the dimension of the system of coupled equations that are remaining to be solved is reduced by two—the coordinate does not appear and the conjugate momentum is constant.

Let $H(t, q, p)$ be a Hamiltonian for some problem with an n-dimensional configuration space and $2n$-dimensional phase space. Suppose the Hamiltonian does not depend upon the ith coordinate

q^i: $(\partial_1 H)_i = 0$.[18] According to Hamilton's equations the conjugate momentum p_i is conserved. Hamilton's equations of motion for the remaining $2n-2$ phase space variables do not involve q^i (because it does not appear in the Hamiltonian), and p_i is a constant. Thus the dimension of the difficult part of the problem, the part that involves the solution of coupled ordinary differential equations, is reduced by two. The remaining equation governing the evolution of q^i in general depends on all the other variables, but once the reduced problem has been solved, then the equation of motion for q^i can be written so as to give Dq^i explicitly as a function of time. We can then find q^i as a definite integral of this function.[19]

Contrast this result with analogous results for more general systems of differential equations. There are two independent situations.

One situation is that we know a constant of the motion. In general, constants of the motion can be used to reduce the dimension of the unsolved part of the problem by one. To see this, let the system of equations be

$$Dz^i = F^i(z^1, z^2, \ldots, z^m) \tag{3.92}$$

where m is the dimension of the system. Assume we know some constant of the motion

$$C(z^1, z^2, \ldots, z^m) = 0. \tag{3.93}$$

At least locally, we expect that we can use this equation to solve for z^m in terms of all the other variables, and use this solution to eliminate the dependence on z^m. The first $m-1$ equations then only depend upon the first $m-1$ variables. The dimension of the system of equations to be solved is reduced by one. After the solution for the other variables has been found, z^m can be found using the constant of the motion.

---

[18] If a Hamiltonian does not depend on a particular coordinate, then sometimes it is said that the Hamiltonian is "cyclic" in that coordinate.

[19] Traditionally, when a problem has been reduced to the evaluation of a definite integral it is said to be reduced to a "quadrature." Thus, the determination of the evolution of a cyclic coordinate q^i is reduced to a problem of quadrature.

Another situation is that one of the variables, say z^i, does not appear in the equations of motion (but there is an equation for Dz^i). In this case the equations for the other variables form an independent set of equations of one dimension less than the original system. After these are solved, then the remaining equation for z^i can be solved by definite integration.

In both situations the dimension of the system of coupled equations is reduced by one. What is different about Hamilton's equations is that these two situations often come together. If a Hamiltonian for a system does not depend on a particular coordinate then the equations of motion for the other coordinates and momenta do not depend on that coordinate. Furthermore, the momentum conjugate to that coordinate is a constant of the motion. An added benefit is that the use of this constant of the motion to reduce the dimension of the remaining equations is automatic in the Hamiltonian formulation. The conserved momentum is a state variable and just a parameter in the remaining equations.

When a generalized coordinate does not appear in the Lagrangian there is some continuous symmetry that is being expressed. The results on the reduction of the phase space show us that in the formulation of a problem for which some symmetry is apparent it will probably be to our advantage if we choose a coordinate system that explicitly incorporates the symmetry, making the Hamiltonian independent of a coordinate. Then the dimension of the phase space of the coupled system will be reduced by two for every coordinate that does not appear in the Hamiltonian.[20]

Motion in a Central Potential

Consider the motion of a particle of mass m in a central potential. A natural choice for the generalized coordinates that reflects the symmetry is polar coordinates. A Lagrangian is (Equation 1.48):

$$L(t;r,\varphi;\dot{r},\dot{\varphi}) = \tfrac{1}{2}m(\dot{r}^2 + r^2\dot{\varphi}^2) - V(r). \tag{3.94}$$

[20]It is not always possible to choose a set of generalized coordinates in which all symmetries are simultaneously manifest. For these systems, the reduction of the phase space is more complicated. We have already encountered such a problem: the motion of a free rigid body. The system is invariant under a rotation about any axis, yet no single coordinate system can reflect this symmetry. Nevertheless, we have already found that the dynamics is described by a system of lower dimension that the full phase space: the Euler equations.

The momenta are $p_r = m\dot{r}$ and $p_\varphi = mr^2\dot{\varphi}$. The kinetic energy is a homogeneous quadratic form in the velocities so the Hamiltonian is $T + V$ with the velocities rewritten in terms of the momenta:

$$H(t; r, \varphi; p_r, p_\varphi) = \frac{p_r^2}{2m} + \frac{p_\varphi^2}{2mr^2} + V(r). \tag{3.95}$$

Hamilton's equations are:

$$\begin{aligned} Dr &= \frac{p_r}{m} \\ D\varphi &= \frac{p_\varphi}{mr^2} \\ Dp_r &= \frac{p_\varphi^2}{mr^3} - DV(r) \\ Dp_\varphi &= 0. \end{aligned} \tag{3.96}$$

The potential energy depends on the distance from the origin, r, as does the kinetic energy in polar coordinates, but neither the potential energy nor the kinetic energy depends on the polar angle φ. The angle φ does not appear in the Lagrangian so we know that p_φ, the momentum conjugate to φ, is conserved along realizable trajectories. The fact that p_φ is constant along realizable paths is expressed by one of Hamilton's equations. That p_φ has a constant value is immediately made use of in the other Hamilton's equations: the remaining equations are a self-contained subsystem with constant p_φ. To make a lower dimensional subsystem in the Lagrangian formulation we have to use each conserved momentum to eliminate one of the other state variables, as we did for the axisymmetric top (see section 2.10).

We can check our derivations with the computer. A procedure implementing the Lagrangian has already been introduced (below Equation 1.48). We can use this to get the Hamiltonian:

```
(show-expression
 ((Lagrangian->Hamiltonian
    (L-central-polar 'm (literal-function 'V)))
  (->H-state 't
             (coordinate-tuple 'r 'phi)
             (momentum-tuple 'p_r 'p_phi))))
```

$$V(r) + \frac{\frac{1}{2}p_\varphi^2}{mr^2} + \frac{\frac{1}{2}p_r^2}{m}$$

and to develop Hamilton's equations:

```
(show-expression
 (((Hamilton-equations
     (Lagrangian->Hamiltonian
       (L-central-polar 'm (literal-function 'V))))
   (coordinate-tuple (literal-function 'r)
                     (literal-function 'phi))
   (momentum-tuple (literal-function 'p_r)
                   (literal-function 'p_phi)))
  't))
```

$$\begin{pmatrix} 0 \\ \begin{pmatrix} Dr(t) - \dfrac{p_r(t)}{m} \\ D\phi(t) - \dfrac{p_\phi(t)}{m(r(t))^2} \end{pmatrix} \\ \begin{bmatrix} Dp_r(t) + DV(r(t)) - \dfrac{(p_\phi(t))^2}{m(r(t))^3} \\ Dp_\phi(t) \end{bmatrix} \end{pmatrix}$$

Axisymmetric top:
We reconsider the axisymmetric top (see section 2.10) from the Hamiltonian point of view. Recall that a top is a rotating rigid body, one point of which is fixed in space. The center of mass is not at the fixed point, and there is a uniform gravitational field. An axisymmetric top is a top with an axis of symmetry. We consider here an axisymmetric top with the fixed point on the symmetry axis.

The axisymmetric top has two continuous symmetries that we would like to exploit. It has the symmetry that neither the kinetic nor potential energy are sensitive to the orientation of the top about the symmetry axis. The kinetic and potential energy are also insensitive to a rotation of the physical system about the vertical axis, because the gravitational field is uniform. We take advantage of these symmetries by choosing coordinates that naturally express them. We already have an appropriate coordinate system that does the job — the Euler angles. We choose the reference orientation of the top so that the symmetry axis is vertical. The first Euler angle ψ expresses a rotation about the symmetry axis. The next Euler angle θ is the tilt of the symmetry axis of the top from the vertical. The third Euler angle φ expresses a rotation of the top about the fixed z axis. The symmetries of the problem imply that the first and third Euler angles do not appear in the Hamiltonian. As a consequence the momenta conjugate to these angles are conserved quantities. The problem of determining the motion of the axisymmetric top is reduced to the problem of determining the evolution of θ and p_θ. Let's work out the details.

In terms of Euler angles, a Lagrangian for the axisymmetric top is (see section 2.10):

```
(define ((L-axisymmetric-top A C gMR) local)
  (let ((q (coordinate local))
        (qdot (velocity local)))
    (let ((theta (ref q 0))
          (thetadot (ref qdot 0))
          (phidot (ref qdot 1))
          (psidot (ref qdot 2)))
      (+ (* 1/2 A
            (+ (square thetadot)
               (square (* phidot (sin theta)))))
         (* 1/2 C
            (square (+ psidot (* phidot (cos theta)))))
         (* -1 gMR (cos theta))))))
```

where gMR is the product of the gravitational acceleration, the mass of the top, and the distance from the point of support to the center of mass. The Hamiltonian is nicer than we have a right to expect:

```
(show-expression
 ((Lagrangian->Hamiltonian (L-axisymmetric-top 'A 'C 'gMR))
  (->H-state 't
             (coordinate-tuple 'theta 'phi 'psi)
             (momentum-tuple 'p_theta 'p_phi 'p_psi))))
```

$$\frac{\frac{1}{2}p_\psi^2}{C} + \frac{\frac{1}{2}p_\psi^2 (\cos(\theta))^2}{A(\sin(\theta))^2} + \frac{\frac{1}{2}p_\theta^2}{A} - \frac{p_\phi p_\psi \cos(\theta)}{A(\sin(\theta))^2} + \frac{\frac{1}{2}p_\phi^2}{A(\sin(\theta))^2} + gMR \cdot \cos(\theta)$$

Note that the angles φ and ψ do not appear in the Hamiltonian, as expected. Thus the momenta p_φ and p_ψ are constants of the motion.

For given values of p_φ and p_ψ we must determine the evolution of θ and p_θ. The Hamiltonian for θ and p_θ is effectively a one degree of freedom Hamiltonian, and this Hamiltonian does not involve the time. Thus the value of the Hamiltonian is conserved along realizable trajectories. This means that the possible trajectories of θ and p_θ can be represented as contours of the Hamiltonian. This gives us a big picture of the possible types of motion and their relationship, for given values of p_φ and p_ψ.

If the top is standing vertically then $p_\varphi = p_\psi$. Let's concentrate first on this case, and let $p = p_\psi = p_\varphi$. For this case the Hamiltonian becomes (after a little trigonometric simplification)

$$H = \frac{p_\theta^2}{2A} + \frac{p^2}{2C} + \frac{p^2}{2A}\tan^2\frac{\theta}{2} + gMR\cos\theta \tag{3.97}$$

Defining the effective potential energy

$$U_{\text{eff}}(\theta) = \frac{p^2}{2C} + \frac{p^2}{2A}\tan^2\frac{\theta}{2} + gMR\cos\theta, \tag{3.98}$$

which parametrically depends on p, A, C, and gMR, the Hamiltonian is

$$H = \frac{p_\theta^2}{2A} + U_{\text{eff}}(\theta). \tag{3.99}$$

If p is large U_{eff} has a single minimum at $\theta = 0$, as we can see in Figure 3.5 For small p there is a minimum for finite positive θ and a symmetrical minimum for negative θ; there is a local maximum at $\theta = 0$. There is a critical value of p at which $\theta = 0$ changes from being a minimum to a local maximum. Denote the critical value by p_c. A simple calculation shows $p_c = \sqrt{4gMRA}$. For $\theta = 0$

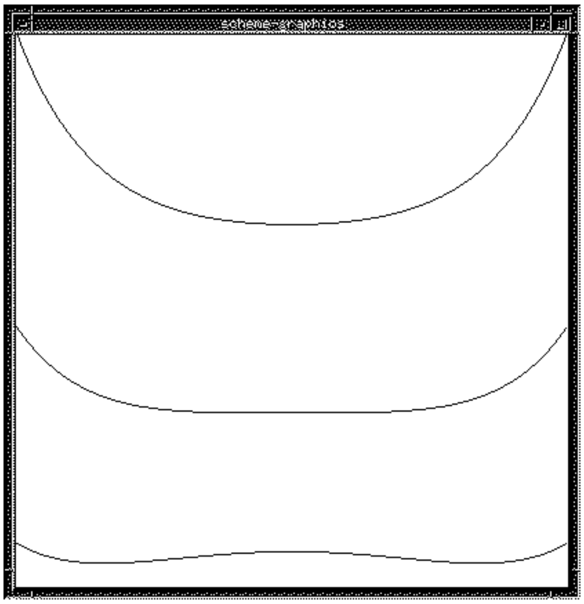

Figure 3.5 The effective potential energy of the axisymmetric top. The effective potential energy, on the ordinate, runs from .02 to .07. The abscissa represents the angle $-\pi/2 < \theta < +\pi/2$. The top curve is for an axial angular momentum $p > p_c$. For this value the top is stable standing vertically. The bottom curve is for $p < p_c$. Here, the top is not stable standing vertically. The middle curve is for p at the critical angular momentum. We see the bifurcation of the stable equilibrium of the sleeping top into three equilibrium points, one of them unstable.

we have $p = C\omega$ where ω is the rotation rate. Thus to p_c there corresponds a critical rotation rate

$$\omega_c = \sqrt{4gMRA}/C. \tag{3.100}$$

For $\omega > \omega_c$ the top can stand vertically; for $\omega < \omega_c$ the top falls if slightly displaced from the vertical. The top which stands vertically is called the "sleeping" top. For a more realistic top friction gradually slows the rotation, and the rotation rate of the top eventually falls below the critical rotation rate and the top "wakes up".

We get additional insight into the sleeping top and the awake top by looking at the trajectories in the θ, p_θ phase plane. The trajectories in this plane are simply contours of the Hamiltonian, because the Hamiltonian is conserved. Figure 3.6 shows a phase portrait for $\omega > \omega_c$. All of the trajectories are loops around the vertical ($\theta = 0$). Displacing the top slightly from the vertical simply places the top on a nearby loop, so the top stays nearly vertical. Figure 3.7 shows the phase portrait for $\omega < \omega_c$. Here the vertical position is an unstable equilibrium. The trajectories which approach the vertical are asymptotic — they take an infinite amount of time to reach it, just as a pendulum with just the right initial conditions can approach the vertical but never reach it. If the top is displaced slightly from the vertical then the trajectories loop around another center with nonzero θ. A top started at the center point of the loop stays there, and one started near this equilibrium point loops stably around it. Thus we see that when the top "wakes up" the vertical is unstable, but the top does not fall to the ground. Rather, it oscillates around a new equilibrium.

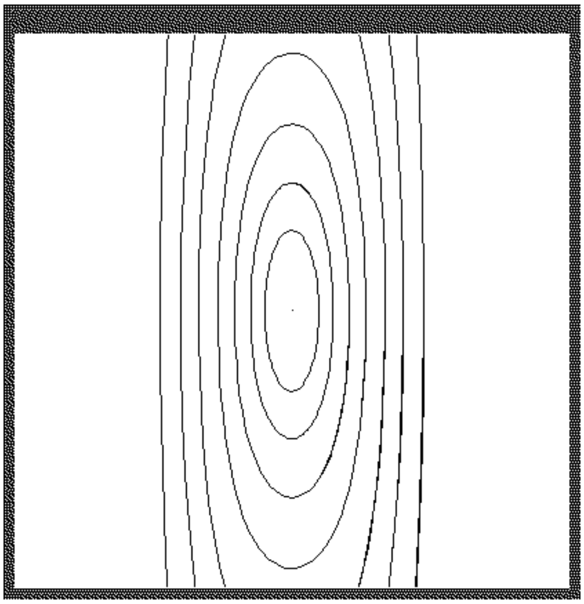

Figure 3.6 The θ, p_θ phase plane for the axisymmetric top with $p_\varphi = p_\psi$ and $\omega = 60$ rad/s. The parameters are $A = 0.0000445\text{kg m}^2$, $C = 0.000025\text{kg m}^2$, $g = 9.8\text{m s}^{-2}$, $M = 0.02$ kg, $R = 0.04$ m. For these parameters the critical frequency ω_c is about 47.25 rad/s. The angle θ, on the abscissa, runs from $-\pi$ to π. The momentum p_θ, on the ordinate, runs from $-0.0005\text{kg m}^2\text{s}^{-1}$ to $0.0005\text{kg m}^2\text{s}^{-1}$.

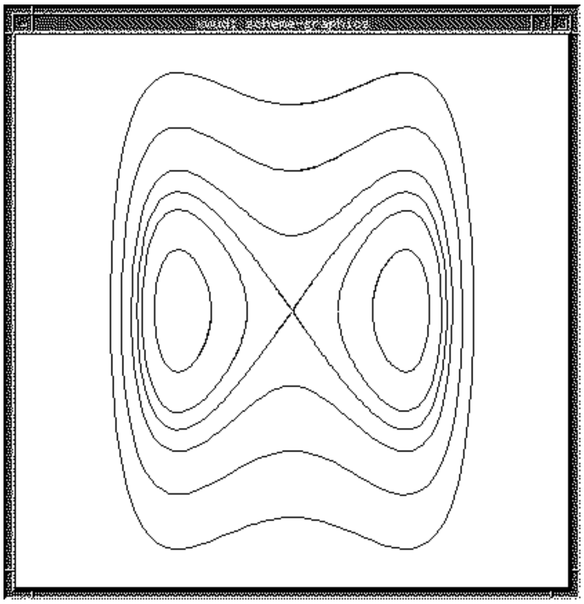

Figure 3.7 The θ, p_θ phase plane for the axisymmetric top with $p_\varphi = p_\psi$ and $\omega = 35$ rad/sec. The momentum p_θ, on the ordinate, runs from $-0.001\text{kgm}^2\text{s}^{-1}$ to $0.001\text{kgm}^2\text{s}^{-1}$. The other parameters are the same as before.

It is also interesting to consider the axisymmetric top when $p_\varphi \neq p_\psi$. Consider the case $p_\varphi > p_\psi$. Some trajectories in the θ, p_θ plane are shown in figure 3.8. Note that in this case trajectories do not go through $\theta = 0$. The phase portrait for $p_\varphi < p_\psi$ is similar and will not be shown.

We have reduced the motion of the axisymmetric top to quadratures by choosing coordinates that express the symmetries. It turns out that the resulting integrals can be expressed in terms of elliptic functions. Thus, the axisymmetric top can be analytically solved. We do not dwell on this solution because it is not very illuminating. In fact, most problems cannot be solved analytically, so there is not much profit in dwelling on the analytic solution of one of the rare problems which is analytically solvable. Rather, our discussion has focused on the geometry of the solutions in the phase space, and the use of integrals to reduce the dimension of the problem. With the phase space portrait we have found some interesting qualitative features of the motion of the top.

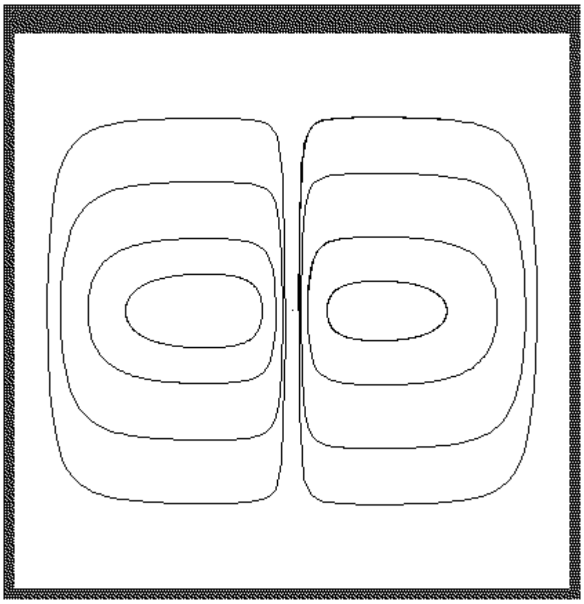

Figure 3.8 The θ, p_θ phase plane for the axisymmetric top with $p_\varphi > p_\psi$. Most of the parameters are the same as before, but here $p_\varphi = 0.0015 \mathrm{kgm}^2\mathrm{s}^{-1}$ and $p_\psi = 0.001 \mathrm{kgm}^2\mathrm{s}^{-1}$. The scale on the ordinate is -0.01 to 0.01 ($\mathrm{kgm}^2\mathrm{s}^{-1}$).

Exercise 3.8: Sleeping Top

Verify that the critical angular velocity above which an axisymmetric top can sleep is given by equation (3.100).

3.5 Phase Space Evolution

Most problems do not have enough symmetries to be reducible to quadrature. It is natural to turn to numerical integration to learn more about the evolution of such systems. The evolution in phase space may be found by numerical integration of Hamilton's equations.

Our numerical integrators take unstructured state; the following procedure takes a Hamiltonian and returns a procedure that takes an integrator state and returns the integrator state derivative.

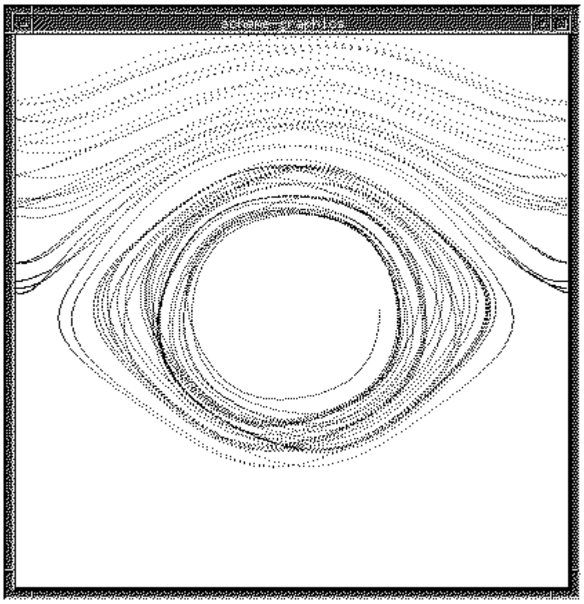

Figure 3.9 This is a phase-space picture of the evolution of the driven pendulum. The phase-space view of the evolution reveals some interesting structure.

```
(define ((Hamiltonian->state-derivative H) istate)
  (let ((H-state (istate->H-state istate)))
    (H-state->istate
      ((phase-space-derivative H) H-state))))
```

As an illustration consider again the periodically driven pendulum (see section 1.6.2). The Hamiltonian is

```
(show-expression
 ((Lagrangian->Hamiltonian
    (L-periodically-driven-pendulum 'm 'l 'g 'a 'omega))
  (->H-state 't 'theta 'p_theta)))
```

$$
\boxed{\begin{aligned}&-\frac{1}{2}a^2 m\omega^2 (\cos(\theta))^2 (\sin(\omega t))^2 + agm\cos(\omega t)\\ &\quad + \frac{a\omega p_\theta \sin(\theta)\sin(\omega t)}{l} - glm\cos(\theta) + \frac{\frac{1}{2}p_\theta^2}{l^2 m}\end{aligned}}
$$

Hamilton's equations for the periodically driven pendulum are unrevealing, so we will not show them. We build a system derivative from the Hamiltonian, and compile it to an executable procedure:

```
(define (H-pend-sysder m l g a omega)
  (Hamiltonian->state-derivative
    (Lagrangian->Hamiltonian
      (L-periodically-driven-pendulum m l g a omega))))

(define H-pend-sysder-compiled
  (compile-parametric 3 H-pend-sysder))
```

Now we integrate this system, given the same initial conditions as in Chapter 1 (see Figure 1.7), but displaying the trajectory in phase space (Figure 3.9).

```
(define (do-it m l g a omega sysder istate0 final-t dt tol)
  (let ((dstate (sysder m l g a omega)))
    (let loop ((istate istate0))
      (let ((H-state (istate->H-state istate)))
        (let ((q ((principal-value pi) (coordinate H-state)))
              (p (momentum H-state)))
          (plot-point window q p))
          (if (< (istate->t istate) final-t)
              (loop (ode-advancer dstate istate dt tol)))))))

(define window (frame -pi pi -10.0 10.0))

(do-it 1.0                         ;m=1kg
       1.0                         ;l=1m
       9.8                         ;g=9.8m/s^2
       0.1                         ;a=1/10 m
       (* 2.0 (sqrt 9.8))          ;omega=2*omega_0
       H-pend-sysder-compiled
       (->istate  0.0              ;t_0=0
                  1.0              ;theta_0=1 radian
                  0.0)             ;p_theta_0= 0.0
       100.0                       ;integrate to 100.0 sec.
       0.01                        ;10000 points
       1.0e-12)                    ;allowable error
```

The trajectory sometimes oscillates and sometimes circulates. The patterns in the phase plane are reminiscent of the trajectories in the phase plane of the undriven pendulum shown in Figure 3.4.

3.5.1 Phase Space Description is Not Unique

We are familiar with the fact that the motion of a system expressed in different coordinate systems is different: the functions that express a motion in rectangular coordinates are different from the functions that express the same motion in polar coordinates. However, with a given coordinate system the evolution of the local state tuple for particular initial conditions is unique. The generalized velocity path function is the derivative of the generalized coordinate path function. On the other hand, the coordinate system alone does not uniquely specify the phase-space description. The relationship of the momentum to the coordinates and the velocities depends on the Lagrangian, and many different Lagrangians may be used to describe the behavior of the same physical system. When two Lagrangians for the same physical system are different the phase-space descriptions of a dynamical state are different.

We have already seen two different Lagrangians for the driven pendulum (see section 1.6.2). One was found using $L = T - V$, and the other was found by inspection of the equations of motion. The two Lagrangians differed by a total time derivative. The momentum p_θ conjugate to θ depends on which Lagrangian we choose to work with, and the description of the evolution in the corresponding phase space also depends on the choice of Lagrangian, even though the behavior of the system is independent of the method used to describe it. The momentum conjugate to θ, using the $L = T - V$ Lagrangian, is

$$p_\theta = ml^2\dot{\theta} - alm\omega \sin\theta \sin\omega t \tag{3.101}$$

and the momentum conjugate to θ, using the alternate Lagrangian, is

$$p_\theta = ml^2\dot{\theta}. \tag{3.102}$$

The two momenta differ by an additive distortion that varies periodically in time and depends on θ. That the phase-space descriptions are different is illustrated in Figure 3.10. The evolution of the system is the same for each.

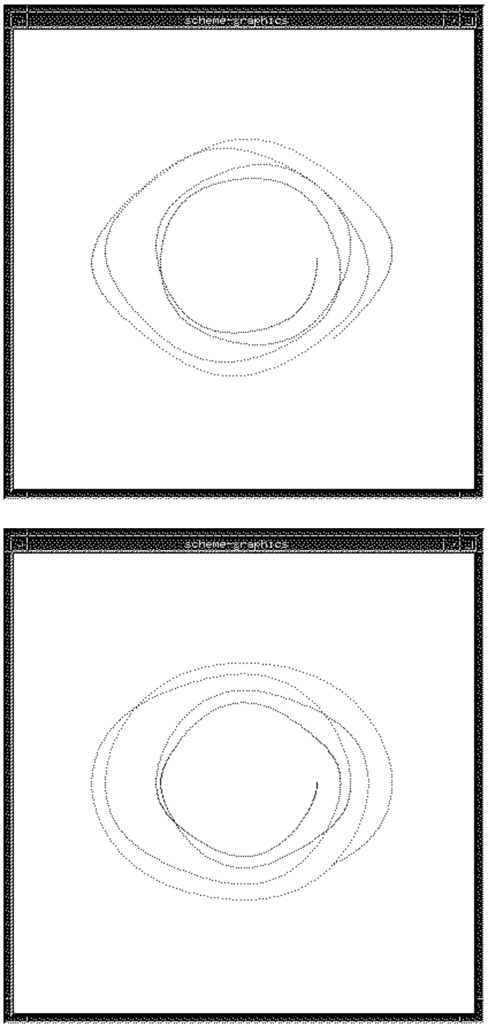

Figure 3.10 An orbit of the driven pendulum in the phase space using $L = T - V$ is shown in the upper plot. In the lower plot the same trajectory is shown in the phase space for the alternate Lagrangian. The evolution is the same, but the phase space representations are not the same.

3.6 Surfaces of Section

Computing the evolution of mechanical systems is just the beginning of understanding the dynamics. Typically, we want to know much more than the phase space evolution of some particular trajectory. We want to obtain a qualitative understanding of the motion. We want to know what sorts of motion are possible, and how one type relates to others. We want to abstract the essential dynamics from the myriad particular evolutions that we can calculate. One tool that we can bring to bear on this problem is a technique called the *surface of section* or *Poincaré section*.[21]

Paradoxically, it turns out that by throwing away most of the calculated information about a trajectory we gain essential new information about the character of the trajectory and its relation to other trajectories. A surface of section is generated by looking at successive intersections of a trajectory or a set of trajectories with a plane in the phase space. Typically, the plane is spanned by a coordinate axis and the canonically conjugate momentum axis. We will see that surfaces of section made in this way have nice properties. The collection of points generated on these surfaces of section reveal important qualitative information about the nature of the trajectories and the relationship among various types of trajectories.[22] The surface of section reveals two qualitatively different types of motion: regular and chaotic. An essential characteristic of the chaotic motions is that initially nearby trajectories separate exponentially with time; the separation of regular trajectories is linear.[23] These two types of trajectories are found

---

[21] The surface of section technique was introduced by Poincaré in his *Méthodes Nouvelles de la Mécanique Céleste*. Poincaré proved remarkable results about dynamical systems using the surface of section technique, and we shall return to those later. The surface of section technique is a key tool in the modern study of dynamical systems, for both analytical and numerical investigations.

[22] The surface of section technique was put to spectacular use in the 1964 landmark paper [11] by astronomers Michel Hénon and Carl Heiles. In their numerical investigations they found that some trajectories are chaotic, and show exponential divergence with time, while other trajectories are regular, showing linear divergence with time. They found that these two types of trajectories are typically clustered in the phase space into regions of chaotic behavior and regions of regular behavior.

[23] That solutions of ordinary differential equations can show exponential sensitivity to initial conditions was independently discovered by Edward Lorenz ([16]) in the context of simplified model of convection in the Earth's

to be clustered in regions of regular motion and regions of chaotic motion.

3.6.1 Poincaré Sections for Periodically-Driven Systems

For a periodically driven system the surface of section is a stroboscopic view of the evolution; we consider only the state of the system at the strobe times, with the period of the strobe equal to the drive period. We generate a surface of section for a periodically-driven system by computing a number of trajectories and accumulating the phase-space coordinates of each trajectory whenever the drive passes through some particular phase. Let T be the period of the drive, then for each trajectory, the surface of section accumulates the phase-space points $(q(t), p(t))$, $(q(t+T), p(t+T))$, $(q(t+2T), p(t+2T))$, and so on (see figure 3.11). If the system has a single degree of freedom, then we can plot the sequence of phase-space points on a q, p surface.

In the case of the stroboscopic section for the periodically driven system the phase of the drive is the same for all section points, thus each phase-space point in the section, with the known phase of the drive, may be considered as an initial condition for the rest of the trajectory. The absolute time of the particular section point does not affect the subsequent evolution; all that matters is that the phase of the drive have the value specified for the section. Thus we can think of the dynamical evolution as generating a map that takes a point in the phase space and generates a new point on the phase space after evolving the system for one drive period. This map of the phase space onto itself is called the *Poincaré map*.

Figure 3.12 shows an example Poincaré section for the driven pendulum. We plot the section points for a number of different initial conditions. We are immediately presented with a new facet of dynamical systems. For some initial conditions, the subsequent section points appear to fill out a set of curves in the section. For other initial conditions this is not the case. Rather, the set of section points appear scattered over a region of the section. In fact, *all* of the scattered points in figure 3.12 were generated from a single initial condition. The surface of section suggests that

atmosphere. Lorenz coined the picturesque term the "butterfly effect" to descibe this sensitivity. The weather system model of Lorenz is so sensitive to initial conditions that "the flapping of a butterfly's wings in Brazil can change the course of a typhoon in Japan."

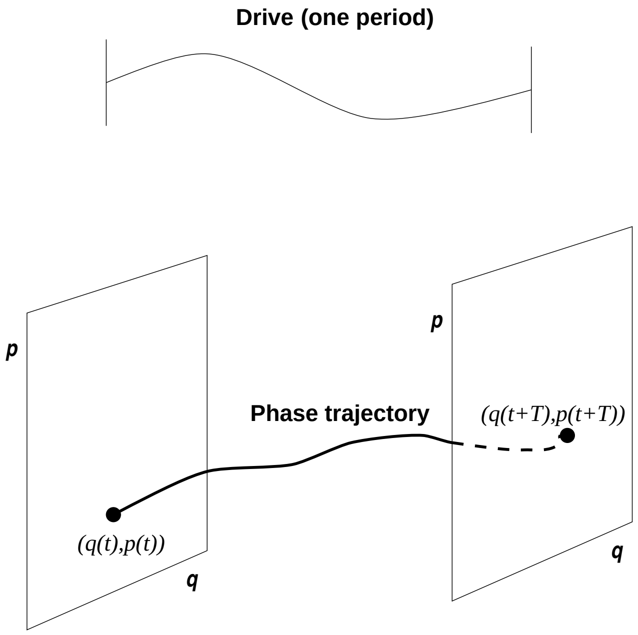

Figure 3.11 Stroboscopic surface of section for a periodically driven system. For each trajectory the surface of section accumulates the set of phase-space points after each full cycle of the drive.

there are qualitatively different classes of trajectories that differ in the dimension of the subspace of the section that they explore.

Trajectories that fill out curves on the surface of section are *regular* trajectories.[24] The curves that are filled out by the regular trajectories are *invariant curves*. They are invariant in that if any section point for a trajectory falls on an invariant curve all subsequent points fall on the same invariant curve. Otherwise stated, the Poincaré map maps every point on an invariant curve onto the invariant curve.

The trajectories that appear to fill areas are termed *chaotic* trajectories. For these points the distance in phase space between initially nearby points grows, on average, exponentially with time.[25] In contrast, for the regular trajectories, the distance in phase space

[24]Regular trajectories are also called *quasiperiodic* trajectories.

[25]We saw an example of this extreme sensitivity to initial conditions in Figure 1.7.

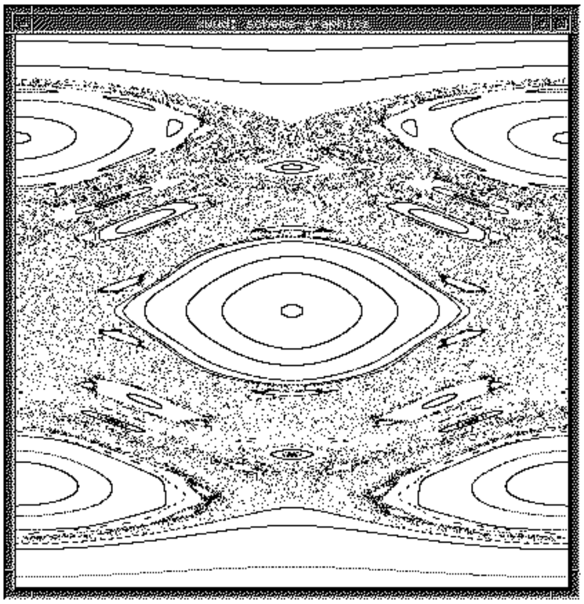

Figure 3.12 Surface of section for the driven pendulum. The angle is plotted on the abscissa (scale $-\pi$ to π); the momentum conjugate to this angle is plotted on the ordinate (scale -20 to 20 kg m^2/s). For this section the parameters are: $m = 1$ kg, $l = 1$m, $g = 9.8$ $\mathrm{m/s}^2$, $A = 0.05$ m, $\omega = 4.2\omega_0$.

between initially nearby points grows, on average, linearly with time.

The phase space seems to be grossly clumped into different regions. Initial conditions in some regions seem to predominately yield regular trajectories, and other regions seem to predominately yield chaotic trajectories. This gross division of the phase space into qualitatively different types of trajectories is called the *divided phase space*. We will see later that there is much more structure here than is apparent at this scale, and that upon magnification there is a complicated interweaving of chaotic and regular regions on finer and finer scales. Indeed, we shall see that many trajectories which appear to generate curves on the surface of section are, upon magnification, actually chaotic and fill a tiny area. We shall also find that there are trajectories which lie on one-dimensional curves on the surface of sction, but which only explore a subset of this curve formed by cutting out an infinite number of holes.[26]

The features seen on the surface of section of the driven pendulum are quite general. The same phenomena are seen in most dynamical systems. In general, there are both regular and chaotic trajectories, and there is the clumping characteristic of the divided phase space. The specific details depend upon the system, but the basic phenomena are generic. Of course we are interested in both aspects: the phenomena which are generic to all systems, and the specific details for particular systems of interest.

The surface of section for the periodically driven pendulum has specific features that give us qualitative information about how this system behaves. The central island in Figure 3.12 is the remnant of the oscillation region for the unforced pendulum (see Figure 3.4). There is a sizable region of regular trajectories here that are, in a sense, similar to the trajectories of the unforced pendulum. In this region, the pendulum oscillates back and forth, much as the undriven pendulum does, but the drive makes it wiggle as it does so. The section points are all collected at the same phase of the drive so we do not see these wiggles on the section.

The central island is surrounded by a large chaotic zone. Thus the region of phase space with regular trajectories similar to the unforced trajectories has finite extent. On the section, the boundary of this "stable" region is apparently rather well defined — there is a sudden transition from smooth regular invariant curves to chaotic motion which can take the system far from this region of regular motion.

There are two other sizeable regions of regular behavior. The trajectories in these regions are resonant with the drive — on average executing one full rotation per cycle of the drive. The two islands differ in the direction of the rotation. In these regions the pendulum is making complete rotations, but the rotation is locked to the drive so that points on the section appear only in the islands with finite angular extent. The fact that points for particular trajectories loop around the islands means that the pendulum sometimes completes a cycle faster than the drive and sometimes slower than the drive, but never loses lock.

[26] One-dimensional invariant sets with an infinite number of holes are sometimes called *cantori*, by analogy to the Cantor sets, but it really doesn't Mather.

Each regular region has finite extent. So from the surface of section we can see directly the range of initial conditions which remain in resonance with the drive. Outside of the regular region initial conditions lead to chaotic trajectories which evolve far from the resonant regions.

Various higher order resonance islands are also visible, as are non-resonant regular circulating orbits. So, the surface of section has provided us with an overview of the main types of motion that are possible and their relationship.

If we change the parameters we can see other interesting phenomena. Figure 3.13 shows the surface of section when the drive frequency is twice the natural small amplitude oscillation frequency of the undriven pendulum. The section has a large chaotic zone, with an interesting set of islands. The central equilibrium has undergone an instability and instead of a central island we find two off-center islands. These islands are alternately visited one after the other. As the support goes up and down the pendulum alternately tips to one side and then the other. It takes two periods of the drive before the pendulum visits the same island. Thus, the system has "period doubled." An island has been replaced by a period-doubled pair of islands. Note that other islands still exist. The islands in the top and bottom of the chaotic zone are the resonant islands, in which the pendulum loops on average a full turn for every cycle of the drive. Note that, as before, if the pendulum is rapidly circulating, the motion is regular.

It is a surprising fact that if we shake the support of a pendulum fast enough then the pendulum can stand upright. This phenomenon can be visualized with the surface of section. Figure 3.14 shows a surface of section when the drive frequency is large compared to the natural frequency. The pendulum can stand upright because there is a regular island at the inverted equilibrium. The surface of section shows that the pendulum can remain upright for a range of initial displacements from the vertical, which can be seen on the surface of section.

3.6.2 Computing stroboscopic surfaces of section

We already have the system derivative for the pendulum, and we can use it to construct a parametric map for constructing Poincaré sections.

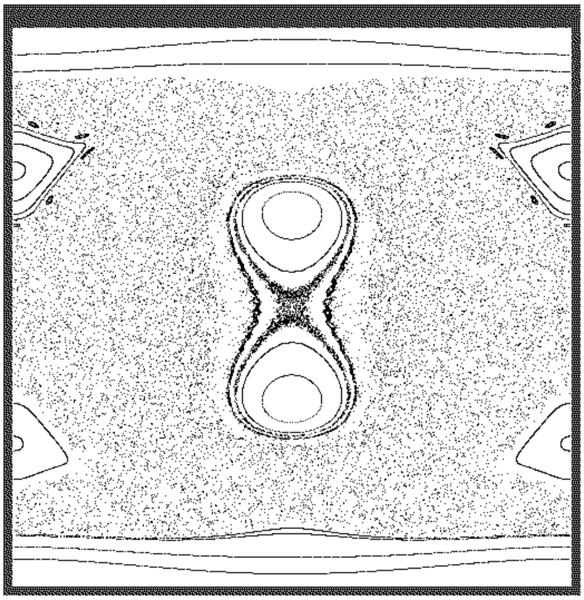

Figure 3.13 Another surface of section for the driven pendulum, illustrating a period-doubled central island. For this section the frequency of the drive is resonant with the frequency of small amplitude oscillations of the undriven pendulum. The angle is plotted on the abscissa (scale $-\pi$ to π); the momentum conjugate to this angle is plotted on the ordinate (scale -10 to 10 kg m^2/s). For this section the parameters are: $m = 1$ kg, $l = 1$ m, $g = 9.8$m/s^2, $A = 0.1$m, $\omega = 2\omega_0$.

```
(define (driven-pendulum-map mass l g a omega)
  (let ((map-period (/ 2pi omega)))
    (lambda (theta p_theta return fail)
      (let ((ns
             (ode-advancer
              (H-pend-sysder-compiled mass l g a omega)
              (->istate          ; state to start from
               0.0               ; t0 = phase/drive-freq
               theta
               p_theta)
              map-period
              1.0e-10)))
        (let ((H-state (istate->H-state ns)))
          (return
           ((principal-value pi) (coordinate H-state))
           (momentum H-state)))))))
```

Figure 3.14 Surface of section for a rapidly driven pendulum, illustrating a vertical equilibrium. The angle is plotted on the abscissa (scale $-\pi$ to π); the momentum conjugate to this angle is plotted on the ordinate (scale -20 to 20 kg m^2/s). For this section the parameters are: $m = 1$ kg, $l = 1$ m, $g = 9.8$ $\mathrm{m/s}^2$, $A = 0.2$ m, $\omega = 10.1\omega_0$.

A map procedure takes the two section coordinates (here `theta` and `p_theta`) and two "continuation" procedures. If the section coordinates given are in the domain of the map, it produces two new section coordinates and passes them to the `return` continuation, otherwise the map procedure calls the `fail` continuation procedure with no arguments.[27]

The trajectories of a map can be explored with an "interactive" interface. The procedure `explore-map` allows us to use a pointing device to choose initial conditions for trajectories. For example, the surface of section in figure 3.12 was generated by plotting a number of trajectories, using a mouse to choose initial conditions, with the following program:

[27]In the particular case of the driven pendulum there is no reason to call `fail`. This contingency is reserved for systems where orbits escape or cease to satisfy some constraint.

```
(define win (frame -pi pi -20 20))

(let* ((m 1.0)                              ;m=1kg
       (l 1.0)                              ;l=1m
       (g 9.8)                              ;g=9.8m/s^2
       (small-amp-freq (sqrt (/ g l)))
       (drive-amplitude 0.05)               ;a=1/20 m
       (drive-frequency
        (* 4.2 small-amp-freq)))
  (explore-map
   win
   (driven-pendulum-map m l g drive-amplitude drive-frequency)
   1000))                     ;1000 points for each IC.
```

Exercise 3.9: Fun with Phase Portraits

Choose some one-degree-of-freedom dynamical system that you are curious about and that can be driven with a periodic drive. Construct a map of the sort we made for the driven pendulum and do some exploring. Are there chaotic regions? Are all of the chaotic regions connected together? Hint: In order for the result to be interesting the system should be nonlinear. It is helpful if the configuration variable is an angle, because this limits its meaningful range.

3.6.3 Poincaré Sections for Autonomous Systems

We illustrated the use of Poincaré sections to visualize qualitative features of the phase space for a one degree-of-freedom system with periodic drive, but the idea is more general. Here we show how Hénon and Heiles used the surface of section to elucidate the properties of an autonomous system.

Hénon-Heiles Background

In the early 60's astronomers were up against a wall. Careful measurements of the motion of nearby stars in the galaxy had allowed particular statistical averages of the observed motions to be determined, and the averages were not at all what was expected. In particular, what was calculated was the velocity dispersion: the root mean square deviation of the velocity from the average. We use angle brackets to denote an average over nearby stars: $\langle w \rangle$ is the average value of some quantity w for the stars in the ensemble. The average velocity is $\langle \dot{\vec{x}} \rangle$. The components of the velocity dispersion are

$$\sigma_x = \langle (\dot{x} - \langle \dot{x} \rangle)^2 \rangle^{1/2} \tag{3.103}$$

$$\sigma_y = \langle (\dot{y} - \langle \dot{y} \rangle)^2 \rangle^{1/2} \tag{3.104}$$

$$\sigma_z = \langle(\dot{z} - \langle\dot{z}\rangle)^2\rangle^{1/2}. \tag{3.105}$$

If we use cylindrical polar coordinates (r, θ, z) and align the axes with the galaxy so that z is perpendicular to the galactic plane and r increases with the distance to the center of the galaxy, then two particular components of the velocity dispersion are:

$$\sigma_z = \langle(\dot{z} - \langle\dot{z}\rangle)^2\rangle^{1/2} \tag{3.106}$$

$$\sigma_r = \langle(\dot{r} - \langle\dot{r}\rangle)^2\rangle^{1/2}. \tag{3.107}$$

It was the expectation at the time that these two components of the velocity dispersion should be equal. In fact they were found to differ by about a factor of 2: $\sigma_r \approx 2\sigma_z$ What was the problem? In the literature at the time there was considerable discussion of what could be wrong. Was the problem some observational selection effect? Were the velocities measured incorrectly? Were the assumptions used in the derivation of the expected ratio not adequately satisfied? For example, the derivation assumed that the galaxy was approximately axisymmetric. Perhaps non-axisymmetric components of the galactic potential were at fault. It turned out that the problem was much deeper. The understanding of motion was wrong.

Let's review the derivation of the expected relation among the components of the velocity dispersion. We wish to give a statistical description of the distribution of stars in the galaxy. We introduce the phase-space distribution function $f(\vec{x}, \vec{p})$ which gives the probability density of finding a star at position $\vec{x}$ with momentum $\vec{p}$.[28] Integrating this density over some finite volume of phase space gives the probability of finding a star in that phase-space volume (in that region of space within a specified region of momenta). We assume the probability density is normalized so that the integral over all of phase space gives unit probability; the star is somewhere and has some momentum with certainty. In terms of f the statistical average of any dynamical quantity w over some volume of phase space V is just

$$\langle w\rangle_V = \int_V fw \tag{3.108}$$

[28]We will see that it is convenient to look at distribution functions in the phase-space coordinates because the consequences of conserved momenta are more apparent, but also because volume in phase space is conserved by evolution.

where the integral extends over the phase-space volume V. In computing the velocity dispersion at some point $\vec{x}$, we would compute the averages by integrating over all momenta.

Individual stars move in the gravitational potential of the rest of the galaxy. It is not unreasonable to assume that the overall distribution of stars in the galaxy does not change much with time, or changes only very slowly. The density of stars in the galaxy is actually very small and close encounters of stars are very rare. Thus, we can model the gravitational potential of the galaxy as a fixed external potential in which individual stars move. The galaxy is approximately axisymmetric. We assume that the deviation from exact axisymmetry is not a significant effect and thus we take the model potential to be exactly axisymmetric.

Consider the motion of a point mass (a star) in an axisymmetric potential (of the galaxy). In cylindrical polar coordinates the Hamiltonian is

$$T + V = \frac{1}{2m}\left[p_r^2 + \frac{p_\theta^2}{r^2} + p_z^2\right] + V(r, z), \tag{3.109}$$

where V does not depend on θ. Since θ does not appear, we know that the conjugate momentum p_θ is constant. For the motion of any particular star we can treat p_θ as a parameter. Thus the effective Hamiltonian has two degrees of freedom

$$\frac{1}{2m}\left[p_r^2 + p_z^2\right] + U(r, z) \tag{3.110}$$

where

$$U(r, z) = V(r, z) + \frac{p_\theta^2}{2mr^2}. \tag{3.111}$$

The value E of the Hamiltonian is constant since there is no explicit time dependence in the Hamiltonian. Thus, we have constants of the motion E and p_θ.

Jeans' "theorem" asserts that the distribution function f depends only on the values of the integrals of motion. That is, we can introduce a different distribution function f' that represents the same physical distribution

$$f'(E, p_\theta) = f(\vec{x}, \dot{\vec{x}}). \tag{3.112}$$

There was good reason to believe that this might be correct. First, it is clear that the distribution function surely depends at least on E and p_θ. The problem is "Given an energy E and angular momentum p_θ what motion is allowed?" The integrals clearly confine the evolution. Does the evolution carry the system everywhere in the phase space subject to these known constraints? In the early part of the 20th century this appeared plausible. Statistical mechanics was successful, and statistical mechanics made exactly this assumption. Perhaps there are other integrals of the motion which exist, but we have not yet discovered them? Poincaré proved an important theorem with regard to integrals of the motion. We shall return to this later, state the theorem more precisely, and prove it for ourselves. For now, the basic idea is that Poincaré proved that most integrals of a dynamical system typically do not persist upon perturbation of the system. That is, if a small perturbation is added to a problem, then most of the integrals of the original problem do not have analogs in the perturbed problem. The integrals are destroyed. Of course, integrals which result from symmetries of the problem continue to be preserved if the perturbed system has the same symmetries. Thus angular momentum continues to be preserved upon application of any axisymmetric perturbation. Poincaré's theorem is correct, but what came next was not. As a corollary to Poincaré's theorem, in 1920 Fermi published a proof of an ergodic theorem, which stated that typically the motion of perturbed problems is ergodic subject to the constraints imposed by the integrals resulting from symmetries. We will define carefully what ergodic means later, but for now it loosely means that trajectories can go everywhere they are allowed to go by the integral constraints. Fermi's theorem was later shown to be incorrect, but on the basis of this theorem we could expect that typically systems fully explore the phase space subject only to the constraints imposed by the integrals resulting from symmetries. Suppose then that the evolution of stars in the galactic potential were subject only to the constraints of conserving E and p_θ. We shall see that this is not true, but if it were we could then conclude that the distribution function for stars in the galaxy can also only depend on E and p_θ.

Given this form of the distribution function, we can deduce the stated ratios of the velocity dispersions. We note that p_z and p_r appear in the same way in the energy. Thus the average of any function of p_z computed with the distribution function must equal the average of the same function of p_r. In particular, the velocity dispersions in the z and r directions must be equal:

$$\sigma_z = \sigma_r. \tag{3.113}$$

But this is not what was observed, which was

$$\sigma_r \approx 2\sigma_z. \tag{3.114}$$

Hénon and Heiles approached this problem differently than others at the time. Rather than improving the models for the motion of stars in the Galaxy, they concentrated on what turned out to be the central issue. What is the qualitative nature of motion? The problem had nothing to do with galactic dynamics in particular, but with the problem of motion. They abstracted the dynamical problem from the particulars of galactic dynamics.

The System of Hénon and Heiles

We have seen that the study of the motion of a point with mass m with an axisymmetric potential energy reduces to the study of a reduced two degree of freedom problem in r and z with potential energy $U(r, z)$. Hénon and Heiles chose to study the motion in a two degree of freedom system with a particularly simple potential energy so the dynamics would be clear and the calculation uncluttered. The Hénon-Heiles Hamiltonian is

$$H(t; x, y; p_x, p_y) = \frac{1}{2}\left(p_x^2 + p_y^2\right) + V(x, y) \tag{3.115}$$

with potential energy

$$V(x, y) = \frac{1}{2}\left(x^2 + y^2\right) + x^2 y - \frac{1}{3}y^3. \tag{3.116}$$

The potential energy is shaped like a distorted bowl. The potential energy has triangular symmetry, which is evident when the potential energy is rewritten in polar coordinates

$$\frac{1}{2}r^2 - \frac{1}{3}r^3 \sin 3\theta. \tag{3.117}$$

Contours of the potential energy are shown in Figure 3.15. At small values of the potential energy the contours are approximately circular; as the value of the potential energy approaches

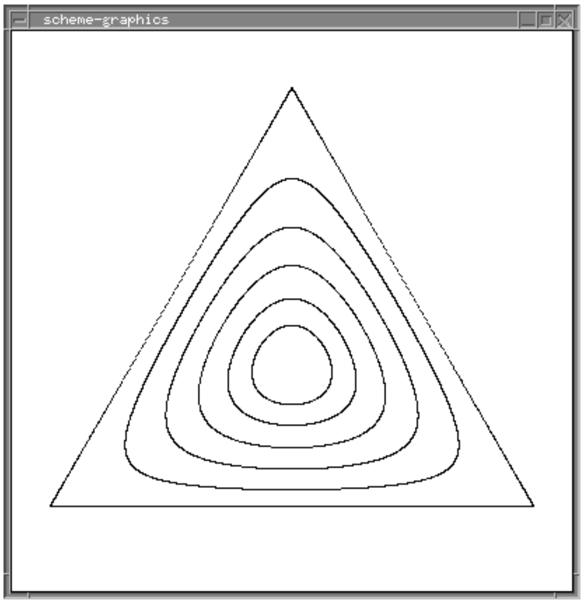

Figure 3.15 Contours of the Hénon-Heiles potential energy. The contours shown, from the inside out, are for potential energies: 1/100, 1/40, 1/20, 1/12, 1/8, and 1/6.

1/6 the contours become triangular, and at larger potential energies the contours open to infinity.

The Hamiltonian is time independent, so energy is conserved. In this case this is the only known integral. We first determine the restrictions that conservation of energy imposes on the evolution. We have

$$E = \frac{1}{2}\left(p_x^2 + p_y^2\right) + V(x, y) \geq V(x, y), \tag{3.118}$$

so the motion is confined to the region inside the contour $V = E$ because the sum of the squares of the momenta cannot be negative.

Let's compute some sample trajectories. For definiteness, we investigate trajectories with energy $E = 1/8$. There are a large variety of trajectories. There are trajectories that circulate in a regular way around the bowl (Figure 3.16), in both directions; there are trajectories that oscillate back and forth (Figure 3.17); there are also trajectories that appear more irregular (Figure 3.18). There

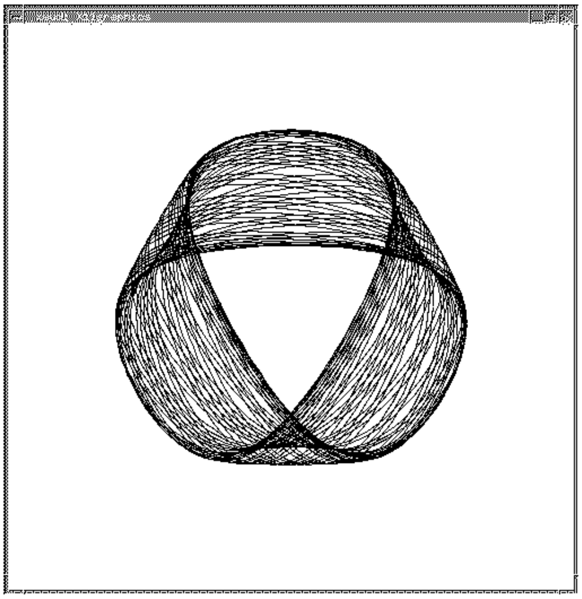

Figure 3.16 A trajectory of the Hénon-Heiles Hamiltonian projected on the (x, y) plane. The energy is $E = 1/8$.

is no end to the trajectories that could be computed, but let's face it, surely there is more to life than looking at trajectories.

The problem facing Hénon and Heiles was the issue of integrals of motion. Are there other integrals besides the obvious ones? They investigated this issue with the surface of section technique. The surface of section is generated by looking at successive passages of trajectories through a plane in phase space. How does this address the issue of the number of integrals? A priori, there appear to be two possibilities: either there are hidden integrals or there are not. Suppose there is no other integral of the motion besides the energy. Then the expectation was that successive intersections of the trajectory with the section plane would eventually explore all of the section plane that is consistent with conservation of energy. On the other hand, if there is a hidden integral then the successive intersections would be constrained to fall on a curve.

Specifically, the surface of section is generated by recording and plotting p_y versus y whenever $x = 0$, as shown in Figure 3.19. Given the value of the energy E and a point (y, p_y) on the section

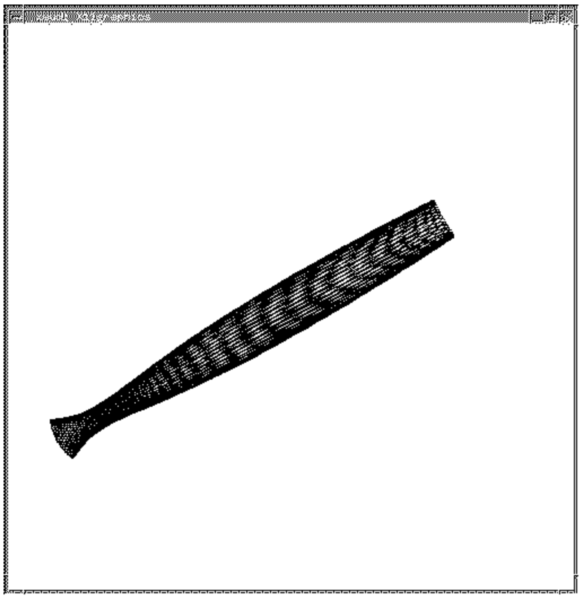

Figure 3.17 Another trajectory of the Hénon-Heiles Hamiltonian projected on the (x, y) plane. The energy is $E = 1/8$.

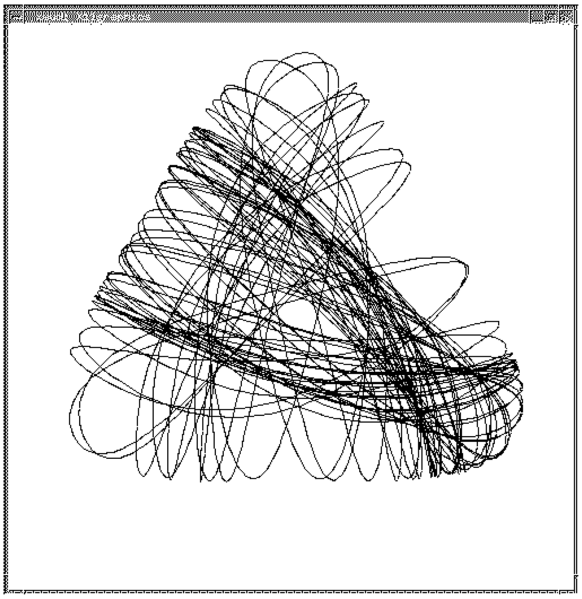

Figure 3.18 Yet another trajectory of the Hénon-Heiles Hamiltonian projected on the (x, y) plane. The energy is $E = 1/8$.

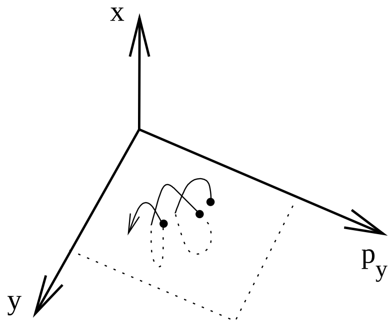

Figure 3.19 The surface of section for the Hénon-Heiles problem is generated by recording and plotting the successive crossings of the $x = 0$ plane in the direction of increasing x.

$x = 0$ we can recover p_x, up to a sign. If we restrict attention to intersections with the section plane that cross with, say, positive p_x, then there is a one to one relation between section points and trajectories. A section point thus corresponds to a unique trajectory.

On the section, the energy is

$$E = H(t; 0, y; p_x, p_y) = \frac{1}{2}\left(p_x^2 + p_y^2\right) + V(0, y) \tag{3.119}$$

Because p_x^2 is positive, the trajectory is confined by the energy integral to regions of the section such that

$$E \geq \frac{1}{2}p_y^2 + V(x = 0, y) \tag{3.120}$$

So, if there is no other integral, we might expect the points on the section to eventually fill the area enclosed by this bounding curve.

On the other hand, suppose there is a hidden extra integral $I(x, y; p_x, p_y) = 0$. Then this integral would provide further constraints on the trajectories and their intersections with the section plane. An extra integral I provides a constraint between the phase-space variables. We can use E to solve for p_x, and on the section $x = 0$, so the extra integral gives a relation between y and p_y on the section. So we expect that if there is another integral the successive intersections of a trajectory with the section plane will fall on a curve.

If there is no extra integral we expect the section points to fill an area; if there is an extra integral we expect the section points to be restricted to a curve. What actually happens? Figure 3.20 shows a surface of section for $E = 1/12$. On the section the section points for several representative trajectories are displayed. By and large, the points appear to be restricted to curves; so there appears to be evidence for an extra integral. Look closely though. Where the "curves" cross, the lines are a little fuzzy. Hmmm.

Let's try a little larger energy $E = 1/8$. The appearance of the section changes qualitatively (Figure 3.21). For some trajectories there still appear to be extra constraints on the motion. But other trajectories appear to fill an area of the section plane, pretty much as we expected of trajectories if there was no extra integral. In particular, all of the scattered points on this section were generated by a single trajectory. Thus, some trajectories behave as if there is an extra integral, and others don't. Wow!

Let's go on to a higher energy $E = 1/6$, just at the escape energy. A section for this energy is shown in Figure 3.22. Now, a single trajectory explores most of the region of the section plane allowed by energy conservation, but not entirely. There are still trajectories that appear to be subject to extra constraints.

We seem to have all possible worlds. At low energy, the system by and large behaves as if there is an extra integral, but not entirely. At intermediate energy, the phase space is divided: some trajectories explore areas whereas others are constrained. At high energy, trajectories explore most of the energy surface; few trajectories show extra constraints. We have just witnessed our first transition to chaos.

There are two qualitatively different types of motion that are revealed by this surface of section, just as we saw in the Poincaré sections for the driven pendulum. There are trajectories which seem to be constrained as if by an extra integral. And there are trajectories that explore an area on the section as though there were no extra integrals. Regular trajectories appear to be constrained by an extra integral to a one-dimensional set on the section; chaotic trajectories are not constrained in this way and explore an area.[29]

[29] As before, upon close examination we may find that trajectories that appear to be confined to a curve on the section are chaotic trajectories which explore a highly confined region. It is known, however, that some trajectories really

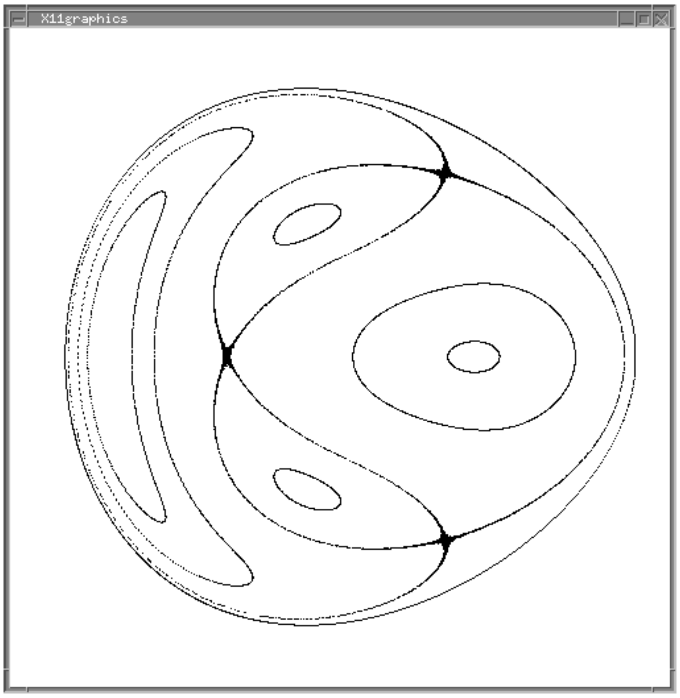

Figure 3.20 Surface of section for the Hénon-Heiles problem with energy $E = 1/12$.

The surface of section not only reveals the existence of qualitatively different types of motion, but it also provides an overview of the different types of trajectories. Take the surface of section for $E = 1/8$ (Figure 3.21). There are four main islands, engulfed in a chaotic sea. The particular trajectories displayed above provide examples from different parts of the section. The trajectory that loops around the bowl (Figure 3.16) belongs to the large island on the left side of the section. Similar trajectories that loop around the bowl in the other direction belong to the large island on the right side of the section. The trajectories that oscillate back and forth across the bowl belong to the two islands above

are confined to curves on the section. Trajectories which start on these curves remain on these curves forever, and the trajectories fill these curves densely. These invariant curves are preserved by the dynamical evolution. We will see that there are also invariant subsets of curves with an infinite number of holes. We will explore the properties of these sets later.

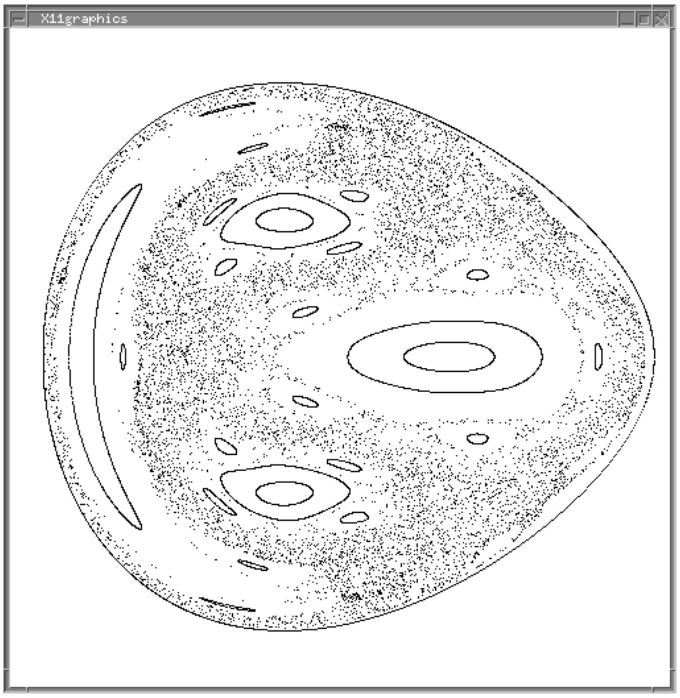

Figure 3.21 Surface of section for the Hénon-Heiles problem with energy $E = 1/8$.

and below the center of the section. (By symmetry there should be three such islands. The third island is snugly wrapped against the boundary of the section.) Each of the main islands is surrounded by a chain of secondary islands. We will see that the types of orbits are inexhaustible, if we look closely enough. The chaotic trajectory (Figure 3.18) lives in the chaotic sea. Thus the section provides a summary of the types of motion possible, and how they are related to one another. It is much more useful than plots of a zillion trajectories.

The sections for various energies summarize the dynamics at that energy. A sequence of sections for various energies shows how the major features change. We have already noticed that at low energy the section is dominated by regular orbits, at intermediate energy the section is divided more or less equally into regular and chaotic regions. At high energies the section is dominated by a single chaotic zone. We will see that such transitions from regular to chaotic behavior are quite common; similar phenomena occur

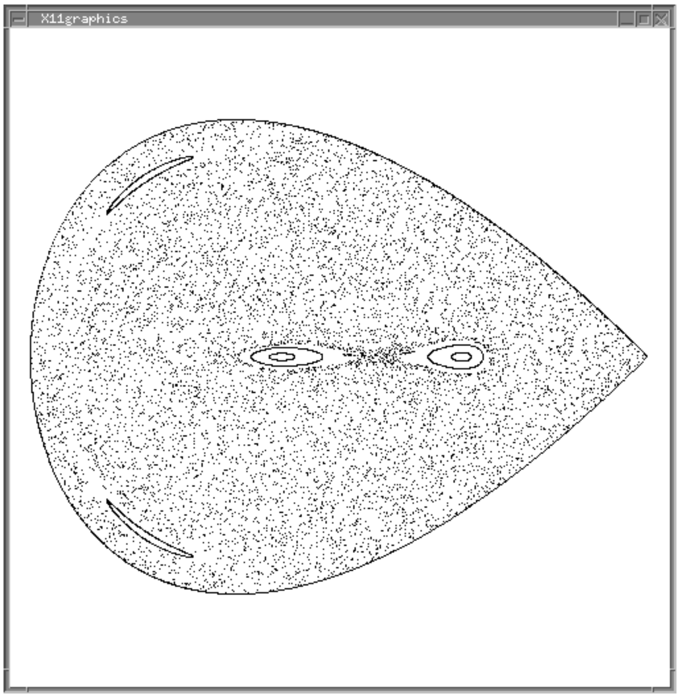

Figure 3.22 Surface of section for the Hénon-Heiles problem with energy $E = 1/6$.

in widely different systems, though the details naturally depend on the system under study.

3.6.4 Non-axisymmetric top

We have seen that the motion an axisymmetric top can be essentially solved. A plot of the rate of change of the tilt angle versus the tilt angle is a simple closed curve. The evolution of the other angles describing the configuration can be obtained by quadrature once the tilting motion has been solved. Now let's consider a non-axisymmetric top. A non-axisymmetric top is a top with three unequal moments of inertia. The pivot is not at the center of mass so uniform gravity exerts a torque. We assume the line between the pivot and the center of mass is one of the principal axes, which we take to be $\hat{c}$. There are no torques about the vertical axis, so the vertical component of the angular momentum is conserved. If we write the Hamiltonian in terms of the Euler an-

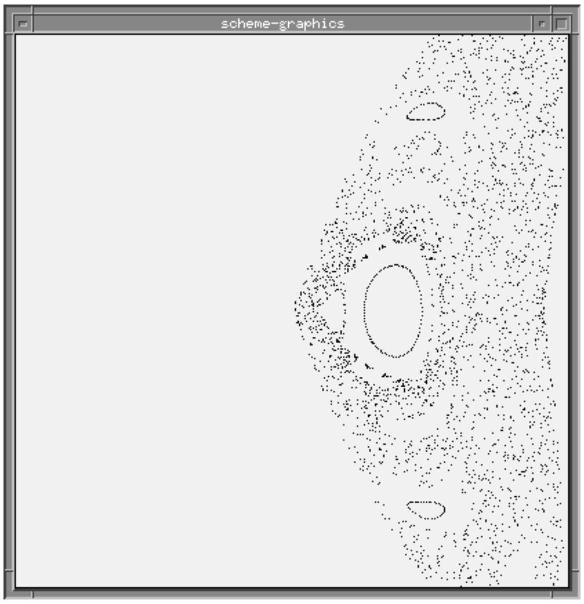

Figure 3.23 A surface of section for the non-axisymmetric top. The parameters are $A = 0.0000445\text{kg m}^2$, $B = 0.000035\text{kg m}^2$, $C = 0.000025\text{kg m}^2$, $g = 9.8\text{m s}^{-2}$, $M = 0.02$ kg, $R = 0.04$m. The energy and p_φ are those of the top initially standing vertically with rotation frequency 35 rad/s. The angle θ, on the abscissa, runs from $-\pi$ to π. The momentum p_θ, on the ordinate, runs from $-0.001\text{kg m}^2\text{s}^{-1}$ to $0.001\text{kg m}^2\text{s}^{-1}$.

gles, the angle φ, which corresponds to rotation about the vertical, does not appear. Thus the momentum conjugate to this angle is conserved. The non-trivial degrees of freedom are θ and ψ, with their conjugate momenta. We can make a surface of section for this problem by displaying p_θ versus θ when $\psi = 0$. There are in general two values of p_ψ possible for given values of energy and p_φ. We plot points only if the value of p_ψ at the crossing is the larger of the two possibilities. This makes the points of the section correspond uniquely to a trajectory.

In Figure 3.23 a surface of section for the non-axisymmetric top is shown. The physical parameters are the same as in Figure 3.7, except that the top is non-axisymmetric. The angular momentum about the center of mass and the energy are the same. What a drastically different picture though!

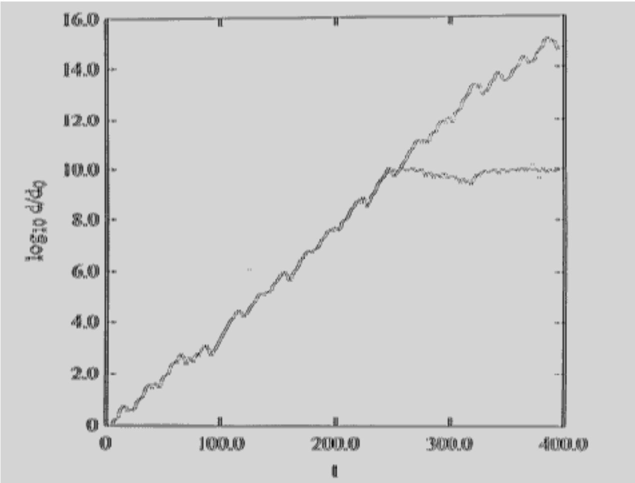

Figure 3.24 The common logarithm of the phase-space distance as a function of time between two chaotic trajectories. The initial distance was 10^{-10}. The logarithm of the distance grows approximately linearly; the distance grows exponentially. The two trajectory method saturates when the distance between trajectories becomes comparable to that allowed by conservation of energy. Also displayed is the distance between trajectories calculated by integrating the linearized variational equations. This method does not saturate.

3.7 Exponential Divergence

Hénon and Heiles discovered that the chaotic trajectories had remarkable sensitivity to small changes in initial conditions—initially nearby chaotic trajectories separate roughly exponentially with time. On the other hand, regular trajectories do not exhibit this sensitivity—initially nearby regular trajectories separate roughly linearly with time.

Consider the evolution of two initially nearby trajectories for the Hénon-Heiles problem, with energy $E = 1/8$. Let $d(t)$ be the usual Euclidean distance in the x, y, p_x, p_y space between the two trajectories at time t. Figure 3.24 shows the common logarithm of $d(t)/d(0)$ as a function of time t. We see that the divergence is well described as exponential.

On the other hand, the distance between two initially nearby regular trajectories grows much more slowly. Figure 3.25 shows the distance between two regular trajectories. The ordinate scale

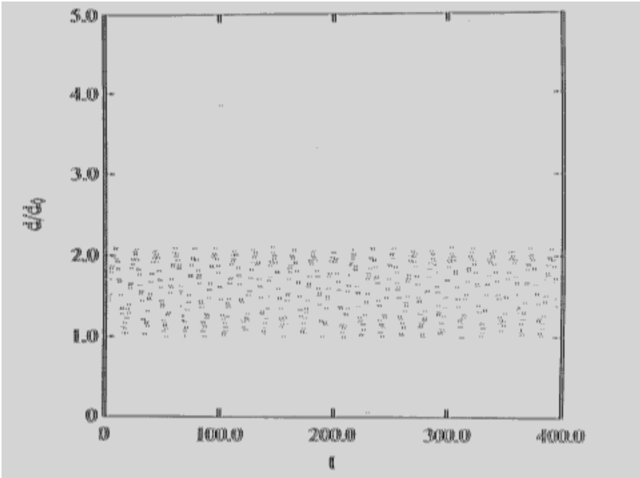

Figure 3.25 The phase-space distance as a function of time between two regular trajectories. The initial distance was 10^{-10}. The distance between the two trajectories oscillates but over this time interval the distance does not grow secularly. In fact, it hardly grows at all.

is linear, and there is basically no secular growth over this time interval.

It is remarkable that Hamiltonian systems have such radically different types of trajectories. On the surface of section the chaotic and regular trajectories differ by the dimension of the space that they explore. It is very interesting that along with this dimensional difference there is a drastic difference in the way chaotic and regular trajectories separate. For higher dimensional systems the surface of technique is not as useful, but trajectories are still distinguished by the way neighboring trajectories diverge: some diverge exponentially whereas others diverge approximately linearly. Exponential divergence is the hallmark of chaotic behavior.

The rate of exponential divergence is quantified by the slope of the graph of $\log(d(t)/d(0))$. We can estimate the rate of exponential divergence of trajectories from a particular phase-space trajectory σ by choosing a nearby trajectory σ' and computing

$$\gamma(t) = \frac{\log(d(t)/d(t_0))}{t - t_0}, \tag{3.121}$$

where $d(t) = \|\sigma'(t) - \sigma(t)\|$. A problem with this method, the "two-trajectory" method, is illustrated in Figure 3.24. For strongly chaotic trajectories two initially nearby trajectories soon find themselves as far apart as they can get. Once this happens the distance no longer grows. The estimate of the rate of divergence of trajectories is limited by this "saturation."

We can improve on this method by studying a variational system of equations. Let

$$Dz(t) = F(t, z(t)) \tag{3.122}$$

be the system of equations governing the evolution of the system. A nearby trajectory z' satisfies

$$Dz'(t) = F(t, z'(t)). \tag{3.123}$$

The difference between these trajectories $\zeta = z' - z$ satisfies

$$D\zeta(t) = F(t, z'(t)) - F(t, z(t)) = F(t, z(t) + \zeta(t)) - F(t, z(t)). \tag{3.124}$$

If ζ is small we can approximate the right-hand side by a derivative

$$D\zeta(t) = \partial_1 F(t, z(t))\zeta(t). \tag{3.125}$$

This set of ordinary differential equations is called the variational equations for the system. It is linear in ζ, and driven by z.

Let $d(t) = \|\zeta(t)\|$, then the rate of divergence can be estimated as before. The advantage of this "variational method" is that w can become arbitrarily large and its growth still measures the divergence of nearby trajectories. We can see in Figure 3.24 that the variational method gives nearly the same result as the two-trajectory method up to the point at which the two-trajectory method saturates.[30]

The *Lyapunov exponent* is defined to be the infinite time limit of $\gamma(t)$, defined by equation (3.121), in which the distance d is computed by the variational method.[31] Actually, for each trajectory there are many Lyapunov exponents, depending on the

---

[30]In strongly chaotic systems w may become so large that the computer can no longer represent it. To prevent this we can replace w by w/c whenever the size of w becomes uncomfortably large. The equation governing w is linear so, except for the scale change, the evolution is unchanged. Of course we have to keep track of these scale changes when computing the average growth rate. This process is called "renormalization" to make it sound impressive.

[31]That this limit exists needs a proof.

initial direction of the variation ζ. For an N dimensional system, there are N Lyapunov exponents. For a randomly chosen $\zeta(t_0)$ the subsequent growth of ζ has components that grow with each of the Lyapunov exponents. In general, however, the growth of w will be dominated by the largest exponent. The largest Lyapunov exponent thus has the interpretation as the typical rate of exponential divergence of nearby trajectories. The sum of the largest two Lyapunov exponents can be interpreted as the typical rate of growth of the area of two-dimensional elements. This can be extended to higher dimensional elements. The rate of growth of volume elements is the sum of all the Lyapunov exponents.

For Hamiltonian systems there are constraints that the Lyapunov exponents must satisfy, which we will justify later. Lyapunov exponents come in pairs: For every Lyapunov exponent λ its negation $-\lambda$ is also an exponent. For every conserved quantity, one of the Lyapunov exponents (and its negation) is zero.[32] So the Lyapunov exponents can be used to check for the existence of conserved quantities. The sum of the Lyapunov exponents for a Hamiltonian system is zero, so volume elements do not exponentially grow. We will see in the next section that phase-space volume is actually conserved for Hamiltonian systems.

3.8 Liouville's Theorem

If an ensemble of states occupies a particular volume of phase space at one moment, then the subsequent evolution of that volume by the flow described by Hamilton's equations may distort the ensemble, but it does not change the volume the ensemble occupies. That phase-space volume is preserved by the phase flow is called *Liouville's Theorem*.

We will first illustrate the preservation of phase-space volume with a simple example and then prove it in general.

Example: the phase flow for the pendulum
Consider an undriven pendulum described by the Hamiltonian:

$$H(t, \theta, p_\theta) = \frac{p_\theta^2}{2l^2 m} + glm \cos\theta. \tag{3.126}$$

[32] This needs a proof.

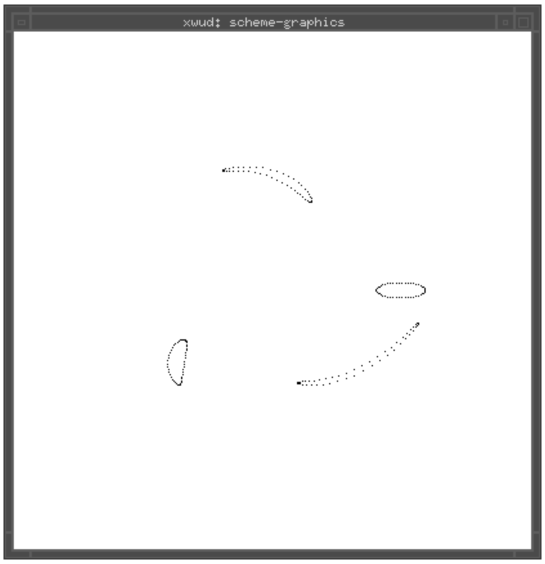

Figure 3.26 A swarm of initial points outlining an area in the phase space of the pendulum deforms as it evolves, but the area contained in the contour remains constant. The horizontal axis is the angle of the pendulum from the vertical in the range $[-\pi, +\pi]$. The vertical axis is the angular momentum in the range $[-10, +10]$ (Joule-seconds). The initial contour is the "ellipse" on the abscissa. The pendulum has length 1 meter in standard gravity (9.8 meter/second^2), so its period is approximately 2 seconds. The flow proceeds clockwise and the deformed areas are shown at .9 seconds, 1.8 seconds, and 2.7 seconds. The successive positions exhibit "shearing" of the region due to the fact that the pendulum is not isochronous for large amplitude motions.

In Figure 3.26 we see the evolution of an elliptic region around a point on the θ-axis, in the oscillation region of the pendulum. Three later positions of the region are shown. The region is stretched and sheared by the flow, but the area is preserved. Because of this we will see that regions become very long and thin. After many cycles, the starting region will be stretched to be a thin layer distributed in the phase angle of the pendulum. Figure 3.27 shows a similar evolution (for smaller time intervals) of a region straddling the separatrix[33] near the unstable equilib-

[33]The separatrix is the curve that separates the oscillating motion from the circulating motion. It is made up of several trajectories that are asymptotic to the unstable equilibrium.

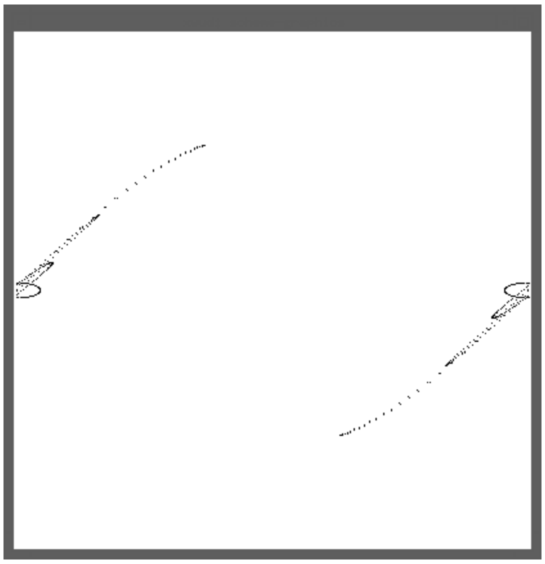

Figure 3.27 The pendulum here is the same as in the previous figure, but now the swarm of initial points surrounds the unstable equilibrium point for the pendulum in phase space, where $\theta = \pi$ and $p_\theta = 0$. The scales of the axes are the same, but here the time interval between successively plotted contours is 0.3 seconds. One clearly sees the phase space stretching out along the separatrix.

rium point. The phase-space region rapidly stretches along the separatrix, while preserving the area. The initial conditions that start in the oscillation region (inside of the separatrix) will continue to spread into a thin ring-shaped region, while the initial conditions that start outside of the separatrix will spread into a thin region of rotation on the outside of the separatrix.

Proof of Liouville's Theorem

Consider a set of ordinary differential equations of the form

$$Dz(t) = F(t, z(t)), \tag{3.127}$$

where z is a tuple of N state variables. Let $R(t_1)$ be a region of the state space at time t_1. Each element of this region is an initial condition at time t_1 for the system. Each element evolves to an element at time t_2 according to the differential equations. The set of these elements at time t_2 is the region $R(t_2)$. Regions evolve to regions.

The evolution of the system for a time interval Δt defines a map $g_{t,\Delta t}$ from the state space to itself:

$$g_{t,\Delta t}(z(t)) = z(t + \Delta t). \tag{3.128}$$

Regions map to regions by mapping each element in the region:

$$g_{t,\Delta t}(R(t)) = R(t + \Delta t). \tag{3.129}$$

The volume $V(t)$ of a region $R(t)$ is $\int_{R(t)} 1$. The volume of the evolved region $R(t + \Delta t)$ is

$$\begin{aligned} V(t + \Delta t) &= \int_{R(t+\Delta t)} 1 \\ &= \int_{g_{t,\Delta t}(R(t))} 1 \\ &= \int_{R(t)} \mathrm{Jac}(g_{t,\Delta t}), \end{aligned} \tag{3.130}$$

where $\mathrm{Jac}(g_{t,\Delta t})$ is the Jacobian of the mapping $g_{t,\Delta t}$. The Jacobian is the determinant of the derivative of the mapping.

For small Δt

$$g_{t,\Delta t}(z(t)) = z(t) + \Delta t F(t, z(t)) + o(\Delta t^2), \tag{3.131}$$

so

$$Dg_{t,\Delta t}(z(t)) = 1 + \Delta t \partial_1 F(t, z(t)) + o(\Delta t^2). \tag{3.132}$$

We can use the fact that if $\mathbf{A}$ is an $N \times N$ square matrix then

$$\det(\mathbf{1} + \epsilon \mathbf{A}) = 1 + \epsilon \operatorname{tr} \mathbf{A} + o(\epsilon^2) \tag{3.133}$$

to show that

$$\mathrm{Jac}(g_{t,\Delta t})(z) = 1 + \Delta t G_t(z) + o(\Delta t^2), \tag{3.134}$$

where

$$G_t(z) = \mathrm{tr}(\partial_1 F(t, z)). \tag{3.135}$$

Thus

$$
\begin{aligned}
V(t+\Delta t) &= \int_{R(t)} \left[1 + \Delta t G_t + o(\Delta t^2)\right] \\
&= V(t) + \Delta t \int_{R(t)} G_t + o(\Delta t^2).
\end{aligned} \tag{3.136}
$$

So the rate of change of the volume at time t is

$$
DV(t) = \int_{R(t)} G_t. \tag{3.137}
$$

Now we compute G_t for a system described by a Hamiltonian H. The components of z are the components of the coordinates and the momenta: $z^k = q^k$, $z^{k+n} = p_k$ for $k = 0, \ldots, n-1$. The components of F are

$$
\begin{aligned}
F^k(t,z) &= (\partial_2 H)^k(t,q,p) \\
F^{k+n}(t,z) &= -(\partial_1 H)_k(t,q,p),
\end{aligned} \tag{3.138}
$$

for $k = 0, \ldots, n-1$. The diagonal components of the derivative $\partial_1 F$ are

$$
\begin{aligned}
(\partial_1)_k F^k(t,z) &= (\partial_1)_k (\partial_2)^k H(t,q,p) \\
(\partial_1)_{k+n} F^{k+n}(t,z) &= -(\partial_2)^k (\partial_1)_k H(t,q,p).
\end{aligned} \tag{3.139}
$$

The component partial derivatives commute, so the diagonal components with index k and index $k+n$ are equal and opposite. We see that the trace, which is the sum of these diagonal components, is zero. Thus the integral of G_t over the region $R(t)$ is zero, so the derivative of the volume at time t is zero. Because t is arbitrary, the volume does not change. This proves *Liouville's theorem*: the phase-space flow conserves phase-space volume.

Notice that the proof of Liouville's theorem does not depend upon whether the Hamiltonian has explicit time dependence. Liouville's theorem holds for systems with time-dependent Hamiltonians.

We may think of the ensemble of all possible states as a fluid flowing around under the control of the dynamics. Liouville's theorem says that this fluid is incompressible for Hamiltonian systems.

Exercise 3.10: Determinants and traces

Show that equation (3.133) is correct.

3.8.1 Area Preservation of Stroboscopic Surfaces of Section

Surfaces of section for periodically driven Hamiltonian systems are area preserving if the section coordinates are the phase space coordinate and momentum. This is an important feature of surfaces of section. It is a consequence of Liouville's theorem for one degree of freedom problems.

It is also the case that surfaces of section such as those we have used for the Hénon-Heiles problem are area preserving, but we are not ready to prove this yet!

3.8.2 Poincaré Recurrence

There is a remarkable theorem which is a trivial consequence of Liouville's theorem — the *Poincaré recurrence theorem.* Loosely, the theorem states that almost all trajectories eventually return arbitrarily close to where they started. This is true regardless of whether the trajectories are chaotic or regular.

More precisely, consider a Hamiltonian dynamical system for which the phase space is a bounded domain D. We identify some initial point in the phase space, say, z_0. Then, for any finite neighborhood U of z_0 that we choose, there are trajectories which emanate from initial points in that neighborhood that eventually return to the neighborhood.

We can prove this by considering the successive images of U under the time evolution. For simplicity, we restrict consideration to time evolution for a time interval Δ. The map of the phase space onto itself generated by time evolution for an interval Δ we call C. Subsequent applications of the map generate a discrete time evolution. Sets of points in phase space transform by evolving all the points in the set; the image of the set U is denoted $C(U)$. Now consider the trajectory of the set U, that is, the sets $C^n(U)$ where C^n indicates the n times composition of C. Now there are two possibilities: either the successive images $C^i(U)$ intersect or they do not. If they do not intersect, then with each iteration, a volume of D equal to the volume of U gets "used up" and cannot belong to the further image. But the volume of D is finite, so we cannot fit an infinite number of non-intersecting finite volumes into it. Therefore, after some number of iterations the images intersect. Suppose, $C^i(U)$ intersects with $C^j(U)$, with $j < i$, for definiteness. Then the preimage of each must also intersect, since the preimage of a point in the intersection belongs to both sets. Thus $C^{i-1}(U)$ intersects $C^{j-1}(U)$. This can be continued until finally we have $C^{i-j}(U)$ intersects U. So we have proven that after $i - j$ iterations of the map C there are a set of points initially in U that return to the neighborhood U.

3.8.3 The Gas in the Corner of the Room

Suppose we have a collection of N classical atoms in a perfectly sealed room. The phase-space dimension of this system is $6N$. A point in this phase space is denoted z. Suppose initially all the atoms are, say, within one centimeter of one corner, with arbitrarily chosen finite velocities. This corresponds to some initial point z_0 in the phase space. The phase space of the system is limited in space by the box, and in momentum by energy conservation; the phase space is bounded. The recurrence theorem then says that in the neighborhood of z_0 there is an initial condition of the system that returns to the neighborhood of z_0 after some time. For the individual atoms this means that after some time all of the atoms will be found in the corner of the room again, and again, and again. Makes one wonder about the second law of thermodynamics, doesn't it?[34]

3.8.4 Non-existence of Attractors in Hamiltonian systems

Some systems have attractors. An *attractor* is a region of phase space that gobbles volumes of trajectories. For an attractor there is some larger region, the basin of attraction, such that sets of trajectories with non-zero volume eventually end up in the attractor and never leave it. The recurrence theorem shows that Hamiltonian systems with bounded phase space do not have attractors. Consider some candidate volume in the proposed basin of attraction. The recurrence theorem guarantees that some trajectories in the candidate volume return to the volume repeatedly. Therefore,

[34]It is reported that when Boltzman was confronted with this problem he responded, "You should wait that long!"

the volume is not in a basin of attraction. Attractors do not exist in Hamiltonian systems with bounded phase space.

This does not mean that every trajectory always returns. A simple example is the pendulum. Suppose we take a blob of trajectories that spans the separatrix, the trajectory that asymptotically approaches the unstable equilibrium with the pendulum pointed up. Trajectories with more energy than the separatrix make a full loop around and return to their initial point; trajectories with lower energy than the separatrix oscillate once across and back to their initial position; but the separatrix trajectory itself leaves the initial region permanently, and continually approaches the unstable point.

3.8.5 Conservation of Phase Volume in a Dissipative System

The definition of a dissipative system is not so clear. For some, "dissipative" implies that phase-space volume is not conserved, which is the same as saying the evolution of the system is not governed by Hamilton's equations. For others, "dissipative" implies friction is present: representing loss of energy to unmodelled degrees of freedom. Here is a curious example. The damped harmonic oscillator is the paradigm of a dissipative system. Here we show that the damped harmonic oscillator can be described by Hamilton's equations and that phase-space volume is conserved.

The damped harmonic oscillator is governed by the ordinary differential equation

$$mD^2x + \alpha Dx + kx = 0 \tag{3.140}$$

where α is a coefficient of damping. We can formulate this system with the Lagrangian [35]

$$L(t, x, \dot{x}) = (\frac{m}{2}\dot{x}^2 - \frac{k}{2}x^2)e^{\frac{\alpha}{m}t}. \tag{3.141}$$

The Lagrange-Euler equation for this is then

$$(mD^2x + \alpha Dx + kx)e^{\frac{\alpha}{m}t} = 0. \tag{3.142}$$

[35] This is just the product of the Lagrangian for the undamped harmonic oscillator with an increasing exponential of time.

Since the exponential is never zero this equation has the same trajectories as equation (3.140) above.

The momentum conjugate to x is

$$p = m\dot{x}e^{\frac{\alpha}{m}t}, \tag{3.143}$$

and the Hamiltonian is

$$H(t, x, p) = (\frac{1}{2m}p^2)e^{-\frac{\alpha}{m}t} + (\frac{k}{2}x^2)e^{\frac{\alpha}{m}t}. \tag{3.144}$$

For this system, the Hamiltonian is not the sum of the kinetic energy of the motion of the mass and the potential energy stored in the spring. The value of the Hamiltonian is not conserved ($\partial_0 H \neq 0$). Hamilton's Equations are

$$\begin{aligned} Dx(t) &= \frac{p(t)}{m}e^{-\frac{\alpha}{m}t} \\ Dp(t) &= -kx(t)e^{\frac{\alpha}{m}t}. \end{aligned} \tag{3.145}$$

Let's consider a numerical case. Let $m = 5, k = 1/4, \alpha = 3$. Here the characteristic roots of the linear constant-coefficient ordinary differential equation (3.140) are $s = -1/10, -1/2$ — an overdamped system. Thus the solutions are

$$\begin{bmatrix} x(t) \\ p(t) \end{bmatrix} = \begin{bmatrix} e^{-\frac{1}{10}t} & e^{-\frac{1}{2}t} \\ -\frac{1}{2}e^{-\frac{1}{2}t} & -\frac{5}{2}e^{-\frac{1}{10}t} \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \end{bmatrix}, \tag{3.146}$$

for A_1 and A_2 determined by the initial conditions:

$$\begin{bmatrix} x(0) \\ p(0) \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ -\frac{1}{2} & -\frac{5}{2} \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \end{bmatrix}. \tag{3.147}$$

Thus we can form the transformation from the initial state to the final state:

$$\begin{bmatrix} x(t) \\ p(t) \end{bmatrix} = \begin{bmatrix} e^{-\frac{1}{10}t} & e^{-\frac{1}{2}t} \\ -\frac{1}{2}e^{-\frac{1}{2}t} & -\frac{5}{2}e^{-\frac{1}{10}t} \end{bmatrix} \begin{bmatrix} 1 & 1 \\ -\frac{1}{2} & -\frac{5}{2} \end{bmatrix}^{-1} \begin{bmatrix} x(0) \\ p(0) \end{bmatrix}. \tag{3.148}$$

The transformation is linear, so the area is transformed by the determinant, which is 1 in this case. Thus, contrary to intuition, the phase-space volume is conserved. So why is this not a contradiction with the statement that there are no attractors in Hamiltonian systems? The answer is that the Poincaré recurrence argument is only true for bounded phase spaces. Here, the momentum expands exponentially with time (as the coordinate contracts), so it is unbounded.

We shouldn't really be too surprised by the way the theory protects itself from an apparent paradox—that the phase volume is conserved even though all trajectories decay to zero velocity and coordinates. The proof of Liouville's theorem allows for time-varying Hamiltonians. In this case we are able to model the dissipation by just such a time-varying Hamiltonian.

Exercise 3.11: Time-Varying Systems

To make the fact that Liouville's theorem holds for time-varying systems even more concrete, extend the results of section 3.8 to show how a swarm of initial points outlining an area in the phase space of the *driven* pendulum deforms as it evolves. Construct pictures analogous to Figures (3.26) and (3.27) for one of the interesting cases where we have surfaces of section. Does the distortion look different in different parts of the phase space? How?

3.8.6 Distribution Functions

We only know the state of a system approximately. It is reasonable to model our state of knowledge by a probability density function on the set of possible states. We often want to know what are the probable consquences, given such incomplete knowledge. As the system evolves, the density function also evolves. Liouville's theorem gives us a handle on this kind of problem.

Let $f(t, q, p)$ be a probability density function on the phase space at time t. For this to be a good probability density function we require that the integral of f over all coordinates and momenta is 1—that the system is somewhere is certain.

There is a set of trajectories that pass through any particular region of phase space at a particular time. These trajectories are neither created nor destroyed, and they proceed as a bundle to another region of phase space at a later time. Liouville's theorem tells us that the volume of the source region is the same as the volume of the target region, so the density must remain constant. Thus $D(f \circ \sigma) = 0$. If we have a system described by the Hamiltonian H then

$$D(f \circ \sigma) = \partial_0 f \circ \sigma + \{f, H\} \circ \sigma. \tag{3.149}$$

so we may conclude that

$$\partial_0 f \circ \sigma + \{f, H\} \circ \sigma = 0. \tag{3.150}$$

This linear partial differential equation governs the evolution of the density function, and thus shows how our state of knowledge evolves.

3.9 Standard Map

We have seen that the surfaces of section for a number of different problems are qualitatively very similar. They all show two qualitatively different types of motion — regular motion and chaotic motion. They show that these types of orbits are clustered — there are regions of the surface of section which have mostly regular trajectories and other regions dominated by chaotic behavior. We have also seen a transition to large-scale chaotic behavior as some parameter is varied. Now we have learned that the map that takes points on a two-dimensional surface of section to new points on the surface of section is area-preserving. The sole property that these maps of the section onto itself have in common (that we know of at this point) is that they preserve area. Otherwise they are quite distinct. Suppose we consider an abstract map of the section onto itself that is area-preserving, without regard for whether the map is generated by some dynamical system. Do area-preserving maps show similar phenomena, or is the dynamical origin of the map crucial to the phenomena we have found?[36]

Consider a map of the phase plane onto itself defined in terms of the dynamical variables θ and its "conjugate momentum" I. The map is

$$I' = (I + K \sin\theta) \bmod 2\pi \tag{3.151}$$

$$\theta' = (\theta + I') \bmod 2\pi. \tag{3.152}$$

[36]This question was also addressed in the remarkable paper by Hénon and Heiles, but with a different map than we use here.

This map is known as the "standard map."[37] A curious feature of the standard map is that the momentum variable I is treated as an angular quantity. The derivative of the map has determinant one, implying the map is area preserving.

We can implement the standard map:

```
(define ((standard-map K) theta I return failure)
  (let ((nI (+ I (* K (sin theta)))))
    (return ((principal-value 2pi) (+ theta nI))
            ((principal-value 2pi) nI))))
```

We use the `explore-map` procedure introduced earlier to use a pointing device to interactively explore the surface of section. For example, to explore the surface of section for parameter $K = 0.6$ we use:

```
(define window (frame 0.0 2pi 0.0 2pi))
(explore-map window (standard-map 0.6) 2000)
```

The resulting surface of section, for a variety of orbits chosen with the pointer are shown in figure 3.28 The surface of section does indeed look qualitatively similar to the surfaces of section generated by dynamical systems.

The surface of section for $K = 1.4$ (as shown in figure 3.29) is dominated by a large chaotic zone. Evidently, the standard map also exhibits a transition to large-scale chaos. So this abstract area-preserving map of the phase plane onto itself shows behavior that is similar to behavior in the sections generated by a Hamiltonian dynamical system. Evidently, the area preservation property of the dynamics in the phase space plays a determining role for many interesting properties of trajectories of mechanical systems.

Exercise 3.12: Fun with Henon's Quadratic Map

Consider the map of the plane defined by the equations:

$x' = x \cos\alpha - (y - x^2) \sin\alpha$

[37] The standard map has been extensively studied. Early investigations were by Chirikov [17] and by Taylor [18]. So the map is sometimes called the Chirikov-Taylor map. Chirikov coined the term "standard map," which we adopt. Of course, there is nothing really "standard" about it, though we will see that it is an approximation, albeit a crude one, to many non-linear resonances.

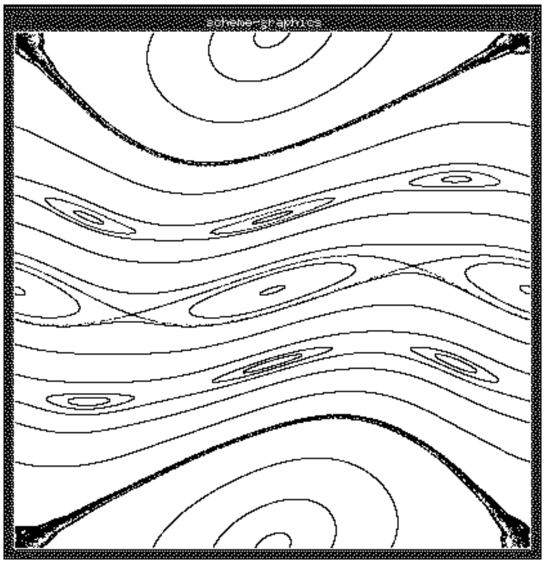

Figure 3.28 Surface of section for the standard map for $K = 0.6$. The section shows mostly regular trajectories, with a few dominant islands, but also shows a number of small chaotic zones.

$$y' = x \sin\alpha + (y - x^2)\cos\alpha$$

a. Show that the map preserves area.

b. Implement the map as a procedure. The interesting range of x and y is $(-1, 1)$. There will be orbits that escape. You should check for values of x and y that escape from this range and call the `fail` continuation when this occurs.

c. Explore the phase portrait of this map for a few values of the parameter α. The map is particularly interesting for $\alpha = 1.32$ and $\alpha = 1.2$. What happens in between?

3.10 Summary

Lagrange's equations are a system of n second order ordinary differential equations in the generalized accelerations, the generalized positions, the generalized velocities, and time. Trajectories are determined by a position and a velocity at a moment.

Hamilton's equations specify the dynamics as a system of first-order ordinary differential equations in the generalized positions,

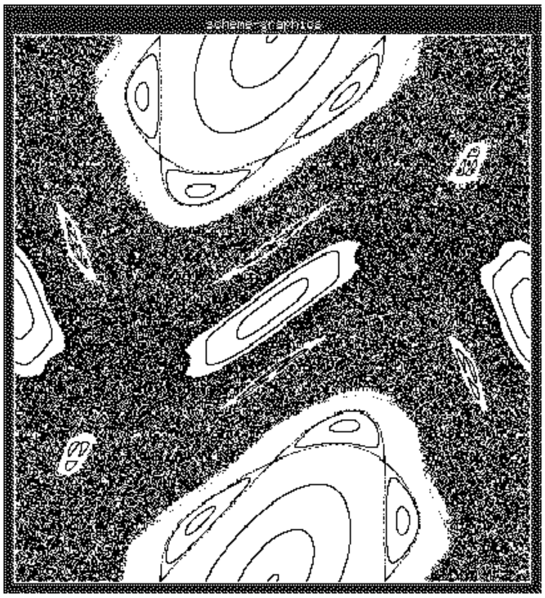

Figure 3.29 Surface of section for the standard map for $K = 1.4$. The dominant feature is a large chaotic zone. There are also some large islands of regular behavior. In this case there are also some interesting secondary islands - islands around islands.

the conjugate momenta, and time. Phase-space trajectories are determined by an initial point in phase space at a moment.

The Hamiltonian formulation and the Lagrangian formulation are equivalent in that equivalent initial conditions produce the same configuration path.

If there is a symmetry of the problem that is naturally expressed as a cyclic coordinate, then the conjugate momentum is conserved. In the Hamiltonian formulation, such a symmetry naturally results in the reduction of the dimension of the phase space of the difficult part of the problem. If there are enough symmetries, then the problem of determining the time evolution may be reduced to evaluation of definite integrals (reduced to quadratures).

Systems without enough symmetries to be reducible to quadratures may be effectively studied with the surface of section technique. This is particularly advantageous in systems for which the reduced problem has two degrees of freedom or has one degree of freedom with explicit periodic time dependence.

Surfaces of section reveal tremendous structure in the phase space. There are chaotic zones and islands of regular behavior. There are interesting transitions as parameters are varied between mostly regular motion to mostly chaotic motion.

Chaotic trajectories exhibit sensitive dependence on initial conditions, separating exponentially from nearby trajectories. Regular trajectories do not show such sensitivity. Curiously, chaotic trajectories are distinguished both by the dimension of the space they explore and by their exponential divergence.

The time evolution of a $2n$-dimensional region in phase space preserves the volume. Hamiltonian flow is "incompressible" flow of the "phase fluid."

Surfaces of section for two degree of freedom systems and for periodically driven one degree of freedom systems are area-preserving. Abstract area-preserving maps of a phase plane onto itself show the same division of the phase space into chaotic and regular regions as surfaces of section generated by dynamical systems. They also show transitions to large-scale chaos.

3.11 Projects

Exercise 3.13: Periodically Driven Pendulum

Explore the dynamics of the driven pendulum, using the surface of section method. We are interested in exploring the regions of parameter space over which various phenomena occur. Consider a pendulum of length 9.8m, mass 1kg, and acceleration of gravity $g = 9.8\mathrm{ms}^{-2}$, giving $\omega_0 = 1\mathrm{rad/s}$. Explore the parameter plane of the amplitude A and frequency ω of the periodic drive.

Examples of the phenomena to be investigated:

a. Inverted equilibrium. Show the region of parameter space (A, ω) in which the inverted equilibrium is stable. If the inverted equilibrium is stable there is some range of stability, i.e. there is a maximum angle of displacement from the equilibrium that stable oscillations reach. If you have enough time, plot contours in the parameter space for different amplitudes of the stable region.

b. Period doubling of the normal equilibrium. For this case, plot the angular positions of the stable and unstable equilibria as functions of the frequency for some given amplitude.

c. Transition to large-scale chaos. Show the region of parameter space (A, ω) for which the chaotic zones around the three principal resonance islands are linked.

Exercise 3.14: Spin-Orbit Surfaces of Section

Write a program to compute surfaces of section for the spin-orbit problem, with the section points being recorded at pericenter. Investigate the following:

a. For out-of-roundness parameter $\epsilon = 0.1$ and eccentricity $e = 0.1$ measure the widths of the regular islands associated with the 1:1, 3:2, and 1:2 resonances.

b. Explore the surfaces of section for a range of ϵ for fixed $e = 0.1$. Estimate the critical value of ϵ above which the main chaotic zones around the 3:2 and the 1:1 resonance islands are merged.

c. For a fixed eccentricity $e = 0.1$ trace the location on the surface of section of the stable and unstable fixed points associated with the 1:1 resonance as a function of the out-of-roundness ϵ.

4
Phase Space Structure

We have seen rather complicated features appear as part of the Poincaré sections of a variety of systems. We have seen fixed points, invariant curves, resonance islands, and chaotic zones in such diverse systems as the driven pendulum, the nonaxisymmetric top, the Hénon-Heiles system, and the spin-orbit coupling of a satellite. Indeed, even in the standard map, where there is no continuous process sampled by the surface of section, the phase space shows similar features.

The motion of other systems is simpler. For some systems conserved quantities can be used to reduce the solution to the evaluation of definite integrals. An example is the axisymmetric top. Two symmetries imply the existence of two conserved momenta, and time independence of the Hamiltonian implies energy conservation. Using these conserved quantities, determining the motion is reduced to the evaluation of definite integrals of the periodic motion of the tilt angle as a function of time. Such systems do not exhibit chaotic behavior; on a surface of section the conserved quantities constrain the points to fall on curves. We may conjecture that if points on a surface of section do not apparently fall on curves then a sufficient number of conserved quantities do not exist to reduce the solution to quadratures.

We have seen a number of instances in which the behavior of a system changes qualitatively as additional effects are added. The free rigid body can be reduced to quadratures, but the addition of gravity gradient torques in the spin-orbit problem yields the familiar mixture of regular and chaotic motions. The motion of an axisymmetric top is also reducible to quadratures, but if the top is made non-axisymmetric then the mixed phase space appears. The system studied by Hénon and Heiles, with the classic mixed phase space, can be thought of as a solvable pair of harmonic oscillators with non-linear coupling terms. The pendulum is solvable, but the driven pendulum has the mixed phase space.

We observe that, as additional effects are turned on, qualitative changes occur in the phase space. Resonance islands appear, chaotic zones appear, some invariant curves disappear, but others persist. Why do resonance islands appear? How does chaotic behavior arise? When do invariant curves persist? Can we draw any general conclusions?

4.1 Emergence of the Mixed Phase Space

We can get some insight into these qualitative changes of behavior by considering systems in which the additional effects are turned on by varying a parameter. For some value of the parameter the system has a sufficient number of conserved quantities to be reducible to quadratures; as we vary the parameter away from this value we can study how the mixed phase space appears. The driven pendulum offers a archetypal example of such a system. If the amplitude of the drive is zero, then solutions of the driven pendulum are the same as the solutions of the undriven pendulum. We have seen surfaces of section for the strongly driven pendulum, illustrating the mixed phase space. Here we crank up the drive slowly and study how the phase portrait changes.

The motion of the driven pendulum with zero amplitude drive is the same as that of an undriven pendulum. The motion of a pendulum was described in section 3.3. Energy is conserved, so all orbits are level curves of the Hamiltonian in the phase plane (see Figure 4.1). There are three regions of the phase plane that have qualitatively different types of motion: the region in which the pendulum oscillates, the region in which the pendulum circulates in one direction, and the region of circulation in the other direction. In the center of the oscillation region there is a stable equilibrium, at which the pendulum is hanging motionless. At the boundaries between these regions the pendulum is asymptotic to the unstable equilibrium, at which the pendulum is standing upright. There are two asymptotic trajectories, corresponding to the two ways the equilibrium can be approached. Each of these is also asymptotic to the unstable fixed point going backward in time.

Driven Pendulum Sections with Zero Drive

Now consider the periodically driven pendulum, but with zero-amplitude drive. The state of the driven pendulum is specified by an angle coordinate, its conjugate momentum, and the phase of the periodic drive. With zero-amplitude drive the evolution of "driven" pendulum is the same as the undriven pendulum. The

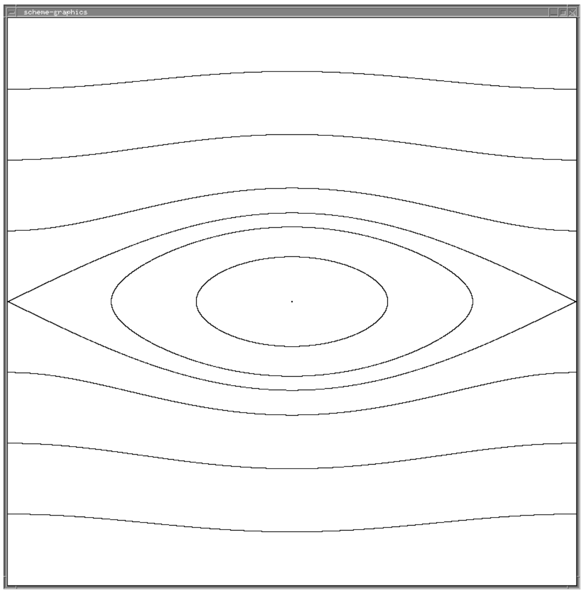

Figure 4.1 The phase plane of the pendulum has three regions displaying two distinct kinds of behavior. Trajectories lie on the contours of the Hamiltonian. Trajectories may oscillate, making ovoid curves around the equilibrium point, or they may circulate, producing wavy tracks outside the eye-shaped region. The eye-shaped region is delimited by the separatrix. This pendulum has length 1m, and the acceleration of gravity is $9.8\mathrm{m\,s^{-2}}$. The abscissa ranges from $-\pi$ to π, and the ordinate runs from $-20\mathrm{kg\,m^2 s^{-1}}$ to $20\mathrm{kg\,m^2 s^{-1}}$.

phase of the drive does not affect the evolution, but we consider the phase of the drive as part of the state so we can give a uniform description that allows us to include the zero-amplitude drive case with the non-zero amplitude case.

For the driven pendulum we make stroboscopic surfaces of section by sampling the state at the drive period, and plotting the angular momentum versus the angle (see Figure 4.2). For zero-amplitude drive, the section points are confined to the curves traced by trajectories of the undriven pendulum. For each kind of orbit that we saw in the one degree of freedom problem, there are orbits of the driven pendulum that generate a corresponding pattern of points on the section.

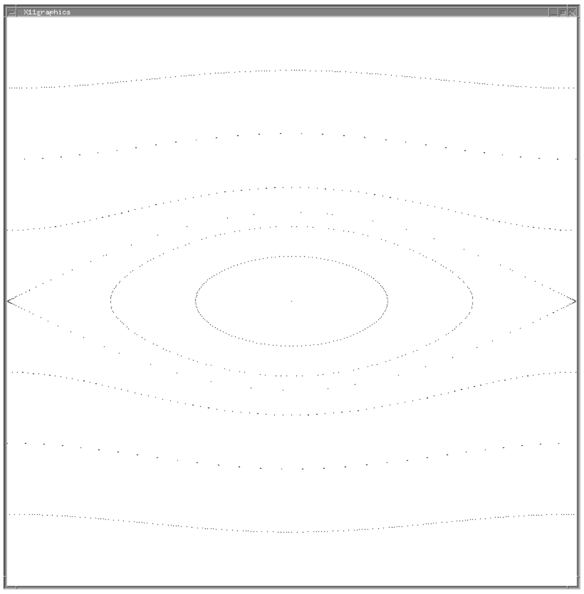

Figure 4.2 A surface of section for the driven pendulum, with zero-amplitude drive. The effect is to sample the trajectories of the undriven pendulum, which lie on the contours of the Hamiltonian. Only a small number of points are plotted for each trajectory to illustrate the fact that for zero-amplitude drive the surface of section samples the continuous trajectories of the undriven pendulum.

The two stationary orbits at the equilibrium points of the pendulum appear as points on the surface of section. Equilibrium points are fixed points of the Poincaré map.

Section points for the oscillating orbits of the pendulum fall on the corresponding contour of the Hamiltonian. Section points for the circulating orbits of the pendulum are likewise confined to the corresponding contour of the Hamiltonian. We notice that the appearance of the points generated by orbits on different contours is different. Typically, if we collected more points on the surface of section the points would eventually fill in the contours. However, there are actually two possibilities. Remember that the period of the pendulum is different for different trajectories. If the period of the pendulum is commensurate with the period of the drive then only a finite number of points will appear on the section. Two periods are commensurate if one is a rational multiple of the other. If the two periods are incommensurate then the section

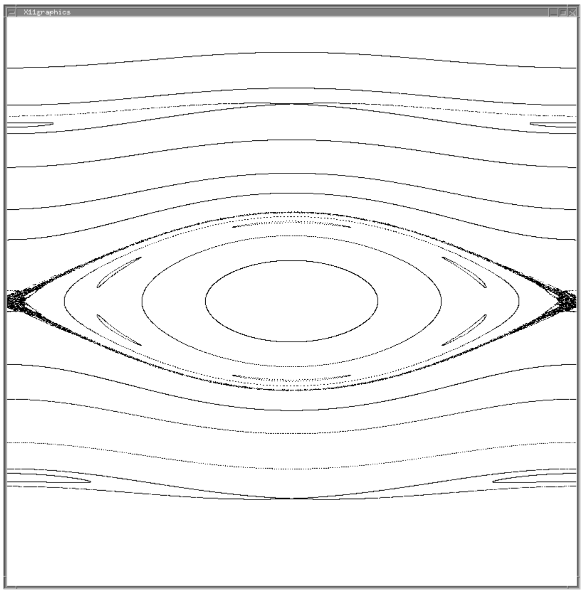

Figure 4.3 A surface of section for the driven pendulum, with nonzero drive amplitude $A = 0.001$m. Many trajectories apparently generate invariant curves, as in the zero-amplitude drive case. Here, in addition, some orbits belong to island chains and others are chaotic. The most apparent chaotic orbit is near the separatrix of the undriven pendulum.

points never repeat. In fact, the points fill the contour densely, coming arbitrarily close to every point on the contour.

Section points for the asymptotic trajectories of the pendulum fall on the contour of the Hamiltonian containing the saddle point. Each asymptotic orbit generates a sequence of isolated points that accumulate near the fixed point. No individual orbit fills the separatrix on the section.

Driven Pendulum Sections for Small Drive

Now consider the surface of section for small drive amplitude (see Figure 4.3). The overall appearance of the surface of section is similar to the section with zero-amplitude drive. Many orbits appear to lie on invariant curves similar to the invariant curves of the zero-drive case. However, there are several new features.

There are now resonance regions that correspond to the pendulum rotating in lock with the drive. These features are found in the upper and lower circulating region of the surface of section.

Each island has a fixed point for which the pendulum rotates exactly once per cycle of the drive. In general, fixed points on the surface of section correspond to periodic motions of the system in the full phase space. The fixed point is at $\pm\pi$, indicating that the pendulum is vertical at the section phase of the drive. For orbits in the resonance region away from the fixed point the points on the section apparently generate curves that surround the fixed point.[1] For these orbits the pendulum rotates on average once per drive, but the phase of the pendulum is sometimes ahead of the drive and sometimes behind it.

There are other islands that appear with non-zero amplitude drive. In the central oscillation region there is a six-fold chain of secondary islands. For this orbit the pendulum is oscillating, and the period of the oscillation is commensurate with the drive. The six islands are all generated by a single orbit. In fact, the islands are visited successively in a clockwise direction. After six cycles of the drive the section point returns to the same island but falls at a different point on the island curve, accumulating the island curve after many iterations. The motion of the pendulum is not periodic, but is locked in a resonance so that on average it oscillates once for every six cycles of the drive.

Another feature which appears is a narrow chaotic region near where the separatrix was in the zero-amplitude drive pendulum. We find that chaotic behavior typically makes its most prominent appearance near separatrices. This is not surprising because the difference in velocities that distinguish whether the pendulum rotates or oscillates is small for orbits near the separatrix. As the pendulum approaches the top, whether it receives the extra nudge it needs to go over the top depends on the phase of the drive.

Actually, the apparent separatrices of the resonance islands for which the pendulum period is equal to the drive period are each generated by a chaotic orbit. To see that this orbit appears to occupy an area one would have to magnify the picture by about a factor of 10^4.

As the drive amplitude is increased the main qualitative changes are the appearance of resonance islands and chaotic zones. Some qualitative characteristics of the zero-case remain. For instance many orbits appear to lie on invariant curves. This behavior is

[1]Keep in mind the abscissa is an angle.

not particular to the driven pendulum; similar features quite generally arise as additional effects are added to problems that are reducible to quadratures. This chapter is devoted to understanding in greater detail how these generic features arise.

4.2 Linear Stability of Fixed Points

Qualitative changes are associated with fixed points of the surface of section. As the drive is turned on chaotic zones appear at fixed points on separatrices of the undriven system, and we observe the appearance of new fixed points associated with resonance islands. Here we investigate the behavior of systems near fixed points. We can distinguish two types of fixed points of a dynamical system. There are fixed points of the differential equations governing the evolution. These are equilibrium points of the system. There are also fixed points on a surface of section. These are either equilibrium points or periodic orbits of the system.

Equilibria of Differential Equations

Consider first the case of a fixed point of a system of differential equations. If a system is initially at an equilibrium point, the system remains there. What can we say about the evolution of the system for points near such an equilibrium point? This is actually a very difficult question, which is not completely answered. We can however understand quite a lot about the motion of systems near equilibrium. The first step is to investigate the evolution of a linear approximation to the differential equations near the equilibrium. This part is easy, and is the subject of linear stability analysis. Later, we will address what the linear analysis implies for the actual problem.

Consider a system of ordinary differential equations

$$Dz(t) = F(t, z(t)), \tag{4.1}$$

with components

$$Dz^i(t) = F^i(t, z^1(t), \ldots, z^n(t)) \tag{4.2}$$

where n is the dimension of the state space. An equilibrium point of this system of equations is a point z_e for which the state derivative is zero:

$$0 = F(t, z_e). \tag{4.3}$$

That this is zero at all moments for the equilibrium solution implies $\partial_0 F(t, z_e) = 0$.

Next consider a state path z' which passes near the equilibrium point. The path displacement ζ is defined so that at time t

$$z'(t) = z_e + \zeta(t). \tag{4.4}$$

We have

$$D\zeta(t) = Dz'(t) = F(t, z_e + \zeta(t)). \tag{4.5}$$

If ζ is small we can write the right-hand side as a Taylor series in ζ:

$$D\zeta(t) = F(t, z_e) + \partial_1 F(t, z_e)\zeta(t) + \cdots, \tag{4.6}$$

but the first term is zero because z_e is an equilibrium point, so

$$D\zeta(t) = \partial_1 F(t, z_e)\zeta(t) + \cdots. \tag{4.7}$$

If ζ is small the evolution is approximated by the linear terms. Linear stability analysis investigates the evolution of the approximate equation

$$D\zeta(t) = \partial_1 F(t, z_e)\zeta(t). \tag{4.8}$$

These are the variational equations (3.125) with the equilibrium solution substituted for the reference trajectory. The relationship of the solutions of this linearized system to the full system is a difficult mathematical problem which is not fully resolved.

If we restrict attention to autonomous systems ($\partial_0 F = 0$) then the variational equations at an equilibrium are a linear system of ordinary differential equations with constant coefficients. Such systems can be solved analytically. To simplify the notation, let $M = \partial_1 F(t, z_e)$, so

$$D\zeta(t) = M\zeta(t). \tag{4.9}$$

We seek a solution of the form

$$\zeta(t) = \alpha e^{\lambda t}, \tag{4.10}$$

where α is a structured constant with the same number of components as ζ. Substituting, we find

$$\lambda \alpha e^{\lambda t} = M \alpha e^{\lambda t}. \tag{4.11}$$

The exponential factor is not zero, so we find

$$M\alpha = \lambda \alpha, \tag{4.12}$$

which is an equation for the eigenvalue λ and (normalized) eigenvector α. In general, there are n eigenvalues and n eigenvectors, so we must add a subscript to both α and λ indicating the particular solution. The general solution is an arbitrary linear combination of these individual solutions. The eigenvalues are solutions of the characteristic equation

$$0 = \det(\mathbf{M} - \lambda \mathbf{I}) \tag{4.13}$$

where $\mathbf{M}$ is the matrix representation of M and $\mathbf{I}$ is the identity matrix of the same dimension. The elements of $\mathbf{M}$ are real, so we know that the eigenvalues λ are either real or come in complex-conjugate pairs. We assume the eigenvalues are all distinct.[2]

If the eigenvalue is real then the solution is exponential, as assumed. If the eigenvalue $\lambda > 0$ then the solution expands exponentially along the direction α; if $\lambda < 0$ then the solution contracts exponentially along the direction α.

If the eigenvalue is complex we can form real solutions by combining the two solutions for the complex-conjugate pair of eigenvalues. Let $\lambda = a + ib$, with real a and b, be one such complex eigenvalue. Let $\alpha = u + iv$, where u and v are real, be the eigenvector corresponding to it. So there is a complex solution of the form

$$\begin{aligned}\zeta_c(t) &= (u + iv)e^{(a+ib)t} \\ &= (u + iv)e^{at}(\cos bt + i \sin bt) \\ &= e^{at}(u \cos bt - v \sin bt)\end{aligned}$$

[2]If the eigenvalues are not unique then the form of the solution is modified.

$$+ ie^{at}(u \sin bt + v \cos bt). \tag{4.14}$$

The complex conjugate of this solution is also a solution, because the ordinary differential equation is linear with real linear coefficients. This complex-conjugate solution is associated with the eigenvalue which is the complex conjugate of the original complex eigenvalue. So the real and imaginary parts of ζ_c are real solutions:

$$\begin{aligned}\zeta_a(t) &= e^{at}(u \cos bt - v \sin bt)\\ \zeta_b(t) &= e^{at}(u \sin bt + v \cos bt)\end{aligned} \tag{4.15}$$

These two solutions reside in the plane containing the vectors u and v. If a is positive both solutions spiral outwards exponentially, and if a is negative they both spiral inwards. If a is zero, both solutions trace the same ellipse, but with different phases.

Again, the general solution is an arbitrary linear combination of the particular real solutions corresponding to the various eigenvalues. So if we denote the k^{th} real eigensolution $\zeta_k(t)$, then the general solution is

$$\zeta(t) = \sum_k A_k \zeta_k(t), \tag{4.16}$$

where A_k may be determined by the initial conditions (the state at a given time).

Exercise 4.1: Pendulum

Carry out the details of finding the eigensolutions for the two equilibria of the pendulum ($\theta = 0$ and $\theta = \pi$, both with $p_\theta = 0$). How is the small amplitude oscillation frequency related to the eigenvalues? How are the eigendirections related to the contours of the Hamiltonian?

Fixed Points of Maps

Fixed points on a surface of section correspond either to equilibrium points of the system or to a periodic motion of the system. Linear stability analysis of fixed points is similar to the linear stability analysis for equilibrium points.

Let T be a map of the state space onto itself, as might be generated by a surface of section. A trajectory sequence is generated by successive iteration of the map T. Let $x(n)$ be the n^{th} point of the sequence. The map carries one point of the trajectory sequence to the next: $x(n+1) = T(x(n))$. We can represent successive iterations of the map by a superscript: so T^i indicates T composed i times. For example, $T^2(x) = T(T(x))$. Thus $x(n) = T^n(x(0))$.

A fixed point x_0 of the map T satisfies

$$x_0 = T(x_0). \tag{4.17}$$

Let x be some trajectory initially near x_0, and ξ be the deviation from x_0: $x(n) = x_0 + \xi(n)$. The trajectory satisfies

$$x_0 + \xi(n+1) = T(x_0 + \xi(n)). \tag{4.18}$$

Expanding the right hand side as a Taylor series we obtain

$$x_0 + \xi(n+1) = T(x_0) + DT(x_0)\xi(n) + \cdots, \tag{4.19}$$

but $x_0 = T(x_0)$ so

$$\xi(n+1) = DT(x_0)\xi(n) + \cdots. \tag{4.20}$$

Linear stability analysis considers the evolution of the system truncated to the linear terms

$$\xi(n+1) = DT(x_0)\xi(n). \tag{4.21}$$

This is a system of linear difference equations, with constant coefficients $DT(x_0)$.

We assume there are solutions of the form

$$\xi(n) = \rho^n \alpha, \tag{4.22}$$

where ρ is some (complex) number. Substituting this solution in the linearized evolution equation we find

$$\rho\alpha = DT(x_0)\alpha, \tag{4.23}$$

or

$$(DT(x_0) - \rho I)\alpha = 0, \tag{4.24}$$

where I is the identity function. We see that ρ is an eigenvalue of the linear transformation $DT(x_0)$, and α is the associated (normalized) eigenvector. Let $M = DT(x_0)$, and $\mathbf{M}$ be its matrix representation. The eigenvalues are determined by

$$\det(\mathbf{M} - \rho\mathbf{I}) = 0. \tag{4.25}$$

The elements of $\mathbf{M}$ are real, so the eigenvalues ρ are either real or come in complex-conjugate pairs.[3]

For the real eigenvalues the solutions are just exponential expansion or contraction along the associated eigenvector α:

$$\xi(n) = \rho^n \alpha. \tag{4.26}$$

The solution is expanding if $\|\rho\| > 1$ and contracting if $\|\rho\| < 1$. If the eigenvalues are complex, then the solution is complex, but the complex solutions corresponding to the complex conjugate pair of eigenvalues can be combined to form two real solutions, as was done for the equilibrium solutions. Let $\rho = \exp(A + iB)$ with real A and B, and $\xi = u + iv$. A calculation similar to that for the equilibrium case show that there are two real solutions

$$\begin{aligned} \xi(n)_a &= \mathrm{e}^{An}\left(u \cos Bn - v \sin Bn\right) \\ \xi(n)_b &= \mathrm{e}^{An}\left(u \sin Bn + v \cos Bn\right). \end{aligned} \tag{4.27}$$

We see that if $A > 0$ then the solution exponentially expands, and if $A < 0$ the solution exponentially contracts. Exponential expansion $A > 0$ corresponds to $\|\rho\| > 1$; exponential contraction corresponds to $\|\rho\| < 1$. If $A = 0$ then the two real solutions and any linear combination of them traces an ellipse.

The general solution is an arbitrary linear combination of each of the eigensolutions. Let ξ_k be the k^{th} real eigensolution. The general solution is

$$\xi(n) = \sum_k A_k \xi_k(n), \tag{4.28}$$

where A_k may be determined by the initial conditions.

Exercise 4.2: Elliptical Oscillation

Show that the arbitrary linear combination of ξ_a and ξ_b traces an ellipse for $A = 0$.

Exercise 4.3: Standard Map

The standard map (see section 3.9) has fixed points at $I = 0$ for $\theta = 0$ and $\theta = \pi$. Find the full eigensolutions for these two fixed points. For what ranges of the parameter K are the fixed points linearly stable or unstable.

---

[3]We assume the eigenvalues are distinct for now.

Relations among exponents

For maps that are generated by stroboscopic sampling of the evolution of a system of autonomous differential equations, equilibrium points are fixed points of the map. The eigensolutions of the equilibrium of the flow and the eigensolutions of the map at the fixed point are then related. Let τ be the sampling period. Then $\rho_i = e^{\lambda_i \tau}$.

The Lyapunov exponent is a measure of the rate of exponential divergence of nearby trajectories from a reference trajectory. If the reference trajectory is an equilibrium of a flow then the Lyapunov exponents are the real parts of the linearized characteristic exponents λ_i. If the reference trajectory is fixed point of a map generated by a flow (either a periodic orbit or an equilibrium) then the Lyapunov exponents are real parts of the logarithm of the characteristic multipliers, divided by the period of the map. So if the characteristic multiplier is $\rho = e^{A+iB}$ and the period of the map is τ then the Lyapunov exponent is A/τ. A positive Lyapunov exponent of a fixed point indicates linear instability of the fixed point.

The Lyapunov exponent has less information than the characteristic multipliers or exponents because the imaginary part is lost. However, the Lyapunov exponent is more generally applicable in that it is well defined even for reference trajectories that are not periodic.

In the linear analysis of the fixed point, each characteristic exponent corresponds to a subspace of possible linear solutions. For instance, for a real characteristic multiplier there is a corresponding eigendirection, and for any initial displacement along this direction successive iterates are also along this direction. Complex-conjugate pairs of multipliers correspond to a plane of solutions. For a displacement initially on this plane, successive iterates are also on this plane.

It turns out that something like this is also the case for the linearized solutions near a reference trajectory that is not at a fixed point. For each non-zero Lyapunov exponent there is a twisting subspace so that for an initial displacement in this subspace successive iterates also belong to the subspace. At different points along the reference trajectory the unit displacement vector that characterizes the direction of this subspace is different.

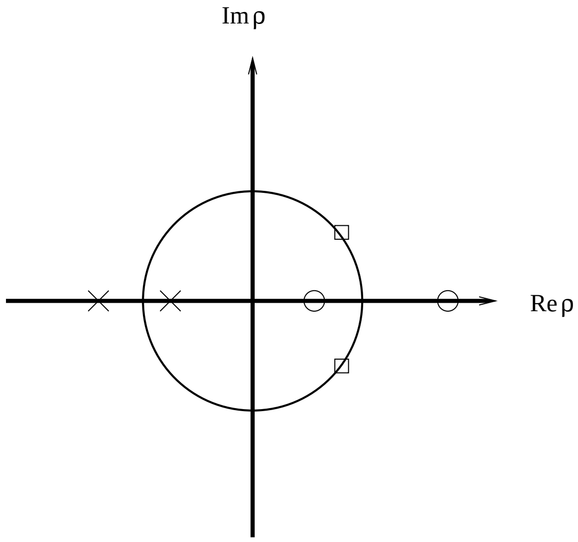

Figure 4.4 The eigenvalues for fixed points of a two-dimensional Hamiltonian map. The eigenvalues are either complex-conjugate pairs that lie on the unit circle or they are real. For each eigenvalue the inverse is also an eigenvalue.

Hamiltonian Specialization

For Hamiltonian systems there are additional constraints among the eigenvalues.

Consider first the case of two-dimensional surfaces of section. We have seen that Hamiltonian surfaces of section are area preserving. As we saw in the proof of Liouville's theorem, area preservation implies that the determinant of the derivative of the transformation is 1. At a fixed point x_0 the linearized map is $\xi(n+1) = DT(x_0)\xi(n)$. So $M = DT(x_0)$ has unit determinant. Now the determinant is the product of the eigenvalues, so for a fixed point on a Hamiltonian surface of section the two eigenvalues must be inverses of each other. We also have the constraint that if an eigenvalue is complex then the complex conjugate of the eigenvalue is also an eigenvalue. These two conditions imply that the eigenvalues must either be real and inverses, or be complex-conjugate pairs on the unit circle (see Figure 4.4).

Fixed points for which the characteristic multipliers all lie on the unit circle are called *elliptic* fixed points. The solutions of the linearized variational equations trace ellipses around the fixed point. Elliptic fixed points are linearly stable.

Fixed points with positive real characteristic multipliers are called *hyperbolic* fixed points. For two-dimensional maps, there is an exponentially expanding subspace and an exponentially contracting subspace. The general solution is a linear combination of these. Fixed points for which the characteristic multipliers are negative are called *hyperbolic with reflection*.

The edge case of two degenerate characteristic multipliers is called *parabolic*. For two degenerate eigenvalues the general solution grows linearly. This happens at points of bifurcation where elliptic points become hyperbolic points or vice versa.

For two-dimensional Hamiltonian maps these are the only possibilities. For higher dimensional Hamiltonian maps, we can get combinations of these: some characteristic multipliers can be real and others complex-conjugate pairs. We might imagine that in addition there would be many other types of fixed points that occur in higher dimension. In fact, there is only one additional type, shown in Figure 4.5. For Hamiltonian systems of arbitrary dimensions it is still the case that for each eigenvalue the complex conjugate and the inverse are also eigenvalues. We can prove this starting from a result that we will prove in Chapter 5. Consider the map of the phase space onto itself that is generated by time evolution of a Hamiltonian system. Let $z = (q, p)$, then the map T_β satisfies $z(t + \beta) = T_\beta(z(t))$ for solutions z of Hamilton's equations. We will show that the derivative of the map T_β is *symplectic*, whether or not the starting point is at a fixed point. A $2n \times 2n$ matrix $\mathbf{M}$ is symplectic if it satisfies

$$\mathbf{M}\mathbf{J}\mathbf{M}^{\mathrm{T}} = \mathbf{J}, \tag{4.29}$$

where $\mathbf{J}$ is the $2n$-dimensional symplectic unit:

$$\mathbf{J} = \begin{bmatrix} \mathbf{0}_{n\times n} & \mathbf{1}_{n\times n} \\ -\mathbf{1}_{n\times n} & \mathbf{0}_{n\times n} \end{bmatrix}, \tag{4.30}$$

with the $n \times n$ unit matrix $\mathbf{1}_{n\times n}$ and the $n \times n$ zero matrix $\mathbf{0}_{n\times n}$.

Using the symplectic property we can show that in general for each eigenvalue its inverse is also an eigenvalue. Assume ρ is an eigenvalue, so ρ satisfies $det(\mathbf{M} - \rho\mathbf{I}) = 0$. This equation

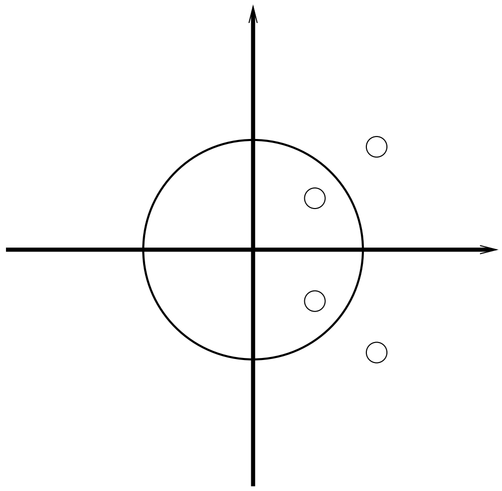

Figure 4.5 If there is more than one degree of freedom the eigenvalues for fixed points of a Hamiltonian map may lie in a quartet, with two complex-conjugate pairs. The magnitudes of the pairs must be inverses. This enforces the constraint that the expansion produced by the roots with magnitude greater than one is counterbalanced by the contraction produced by the roots with magnitude smaller than one.

is unchanged if $\mathbf{M}$ is replaced by its transpose, so ρ is also an eigenvalue of $\mathbf{M}^{\mathrm{T}}$:

$$\mathbf{M}^{\mathrm{T}}\boldsymbol{\alpha}' = \rho\boldsymbol{\alpha}'. \tag{4.31}$$

From this we can see that

$$\frac{1}{\rho}\boldsymbol{\alpha}' = (\mathbf{M}^{\mathrm{T}})^{-1}\boldsymbol{\alpha}'. \tag{4.32}$$

Now, from the symplectic property we have

$$\mathbf{MJ} = \mathbf{J}(\mathbf{M}^{\mathrm{T}})^{-1}. \tag{4.33}$$

So

$$\mathbf{MJ}\boldsymbol{\alpha}' = \mathbf{J}(\mathbf{M}^{\mathrm{T}})^{-1}\boldsymbol{\alpha}' = \frac{1}{\rho}\mathbf{J}\boldsymbol{\alpha}', \tag{4.34}$$

and we can conclude that $1/\rho$ is an eigenvalue of $\mathbf{M}$ with the eigenvector $\mathbf{J}\boldsymbol{\alpha}'$. From the fact that for every eigenvalue its inverse is also an eigenvalue we deduce that the determinant of the transformation $\mathbf{M}$, which is the product of the eigenvalues, is one.

The constraints that the eigenvalues must be associated with inverses and complex conjugates yields exactly one new pattern of eigenvalues in higher dimensions. Figure 4.5 shows the only new pattern that is possible.

We have seen that the Lyapunov exponents for fixed points are related to the characteristic multipliers for the fixed points, so the Hamiltonian constraints on the multipliers correspond to Hamiltonian constraints for Lyapunov exponents at fixed points. For each characteristic multiplier, the inverse is also a characteristic multiplier. This means that at fixed points, for each positive Lyapunov exponent there is a corresponding negative Lyapunov exponent with the same magnitude. It turns out that this is also true if the reference trajectory is not at a fixed point. For Hamiltonian systems, for each positive Lyapunov exponent there is a corresponding negative exponent of equal magnitude.

Exercise 4.4: Quartet

Describe (perhaps by drawing cross sections) the orbits that are possible with quartets.

4.3 Homoclinic Tangle

For the driven pendulum we observe that as the amplitude of the drive is increased the separatrix of the undriven pendulum is where the most prominent chaotic zone appears. Here we examine the motion in the vicinity of the separatrix of the undriven pendulum in great detail. What emerges is a remarkably complicated picture, first discovered by Henri Poincaré. Indeed, Poincaré stated that the picture that had emerged was so complicated that he was not even going to attempt to draw it. We will review the argument leading to the picture, and compute enough of it to convince ourselves of its reality.

The separatrix of the undriven pendulum is made up of two trajectories that are asymptotic to the unstable equilibrium. In the driven pendulum with zero drive, there are an infinite number of distinct orbits that lie on the separatrix, which are distinguished

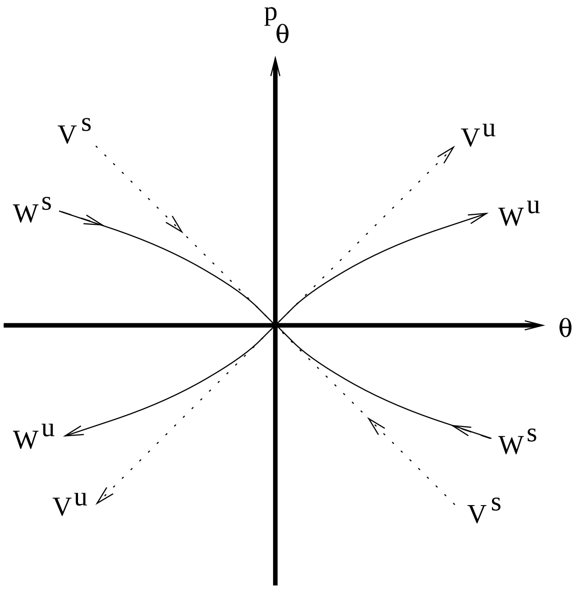

Figure 4.6 The neighborhood of the unstable fixed point of the pendulum shows the stable and unstable manifolds of the nonlinear pendulum and of the linearized variational system around the fixed point. The axes are centered at the fixed point $(\pm\pi, 0)$. The linear stable and unstable manifolds are labeled by V^s and V^u; the nonlinear stable and unstable manifolds are labeled by W^s and W^u.

by the phase of the drive. These orbits are asymptotic to the unstable fixed point both forward and backward in time.

Notice that close to the unstable fixed point the sets of points that are asymptotic to the unstable equilibrium must be tangent to the linear variational eigenvectors at the fixed point. (See Figure 4.6.) In a sense, the sets of orbits that are asymptotic to the fixed point are extensions to the non-linear problem of the sets of orbits that are asymptotic to the fixed point in the linearized problem.

In general, the set of points that are asymptotic to a fixed point forward in time is called the *stable manifold* of the fixed point. The set of points that are asymptotic to a fixed point backward in time is called the *unstable manifold.* For the driven pendulum with zero amplitude drive all points on the separatrix are asymptotic both forward and backward in time to the unstable fixed point. So in this case the stable and unstable manifolds coincide.

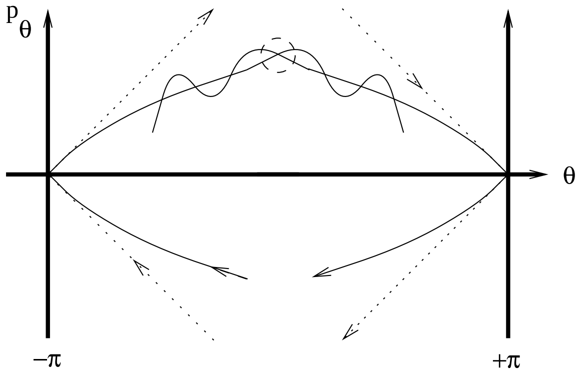

Figure 4.7 For non-zero drive the stable and unstable manifolds no longer coincide and in general cross. The dashed circle indicates the central intersection. Forward and backward images of this intersection are themselves intersections. Because the orbits are asymptotic to the fixed point there are an infinity of such intersections.

If the drive amplitude is non-zero then there are still one-dimensional sets of points that are asymptotic to the unstable fixed point forward and backward in time: there are still stable and unstable manifolds. Why? The behavior near the fixed point is described by the linearized variational system. For the linear variational system, points in the space spanned by the unstable eigenvector, when mapped backwards in time, are asymptotic to the fixed point. Points slightly off this curve may initially approach the unstable equilibrium, but eventually will fall away to one side or the other. For the driven system with small drive, there must still be a curve which separates the points that fall away to one side from the points that fall away to the other side. Points on the dividing curve must be asymptotic to the unstable equilibrium. The dividing set cannot have positive area because the map is area preserving.

In general, for non-zero drive the stable manifolds and unstable manifolds no longer coincide. For the zero-amplitude drive case the stable and unstable manifolds are contours of the conserved Hamiltonian. For non-zero amplitude the Hamiltonian is no longer conserved.

If the stable and unstable manifolds no longer coincide where do they go? In general, the stable and unstable manifolds must cross one another. The only other possibilities are that they run off to infinity or spiral around. Area preservation can be used to exclude the spiraling case. We will see that in general there are barriers to running away. So the only possibility is that the stable and unstable manifolds cross. This is illustrated in Figure 4.7. The point of crossing of a stable and unstable manifold is called a *homoclinic intersection* if the stable and unstable manifolds belong to the same unstable fixed point. It is called a *heteroclinic intersection* if the stable and unstable manifolds belong to different fixed points.

If the stable and unstable manifolds cross once then there are an infinite number of other crossings. The intersection point belongs to both the stable and unstable manifolds. That it is on the unstable manifold means that all images forward and backward in time also belong to the unstable manifold, and likewise for points on the stable manifold. Thus all images of the intersection belong to both the stable and unstable manifolds. So these images must be additional crossings of the two manifolds.

We can deduce that there are still more intersections of the stable and unstable manifolds. The maps we are considering not only preserve area, but they preserve orientation. In the proof of Liouville's theorem we showed that the determinant of the transformation is one, not just magnitude one. If we consider little segments of the stable and unstable manifolds near the intersection point then these segments must map near the image of the intersection point. That the map preserves orientation implies that the manifolds are crossing one another in the same sense as at the previous intersection. Therefore there must have been at least one more crossing of the stable and unstable manifolds in between these two. This is illustrated in Figure 4.8. Of course, all forward and backward images of these intermediate intersections are also intersections.

As the picture gets more complicated keep in mind that the stable manifold cannot cross itself and the unstable manifold cannot cross itself. Suppose one did, say by making a little loop. The image of this loop under the map must also be a loop. So if there was a loop there would have to be an infinite number of loops. That would be ok, but what happens as the loop gets close to the fixed point? There would still have to be loops, but then the stable and unstable manifolds would not have the right behavior. The stable and unstable manifolds of the linearized map do not

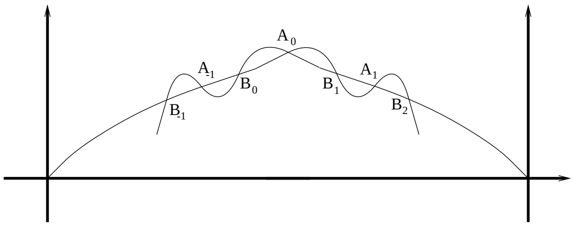

Figure 4.8 Orientation preservation implies that between an intersection of the stable and unstable manifolds and the image of this intersection there is another intersection. Thus there are two alternating families of intersections. The central intersection and its pre- and post-images are labeled A_i. Another family is labelled B_i.

have loops. Therefore, the stable and unstable manifolds cannot cross themselves.[4]

We are not done yet! The lobes that are defined by successive crossings of the stable and unstable manifolds enclose a certain area. The map is area preserving so all images of these lobes must have the same area. So there are an infinite number of images of these lobes, all with the same area. Furthermore, the boundaries of these images cannot cross. As the lobes approach the fixed point we get an infinite number of lobes with a base with an exponentially shrinking length. In order to pack these together on the plane, without the boundaries crossing each other, the lobes must stretch out to preserve area. We see that the length of the lobe must grow roughly exponentially (It may not be uniform in width so it need not be exactly exponential.) This exponential lengthening of the lobes no doubt bears some responsibility for the exponential divergence of nearby trajectories of chaotic orbits, but does not prove it. It does however suggest a connection between the fact that chaotic orbits appear to occupy an area on the section and the fact that nearby chaotic orbits diverge exponentially.

Actually, the situation is even more complicated. As the lobes stretch, they form tendrils that wrap around the separatrix region. The tendrils of the unstable manifold can cross the tendrils of the

[4]Sometimes it is argued that the stable and unstable manifolds cannot cross themselves on the basis of the uniqueness of solutions of differential equations. This is an incorrect argument. The stable and unstable manifolds are not themselves solutions of a differential equation, they are sets of points whose solutions are asymptotic to the unstable fixed points.

stable manifold. Each point of crossing is a new homomclinic intersection, and so each pre and post image of this point belongs to both the stable and unstable manifolds, indicating another crossing of these curves. We could go on and on. No wonder Poincaré refused to draw this mess.

Exercise 4.5: Homoclinic Paradox

How do we fit an infinite number of copies of a finite area in a finite region, without allowing the stable and unstable manifolds to cross themselves? Resolve this apparent paradox.

Computation of Stable and Unstable Manifolds

The homoclinic tangle is not just a bad dream. We can actually compute it.

Very close to an unstable fixed point the stable and unstable manifolds become indistinguishable from the rays along the eigenvectors of the linearized system. So one way to compute the unstable manifold is to take a line of initial conditions close to the fixed point along the unstable manifold of the linearized system and evolve them forward in time. Similarly, the stable manifold can be constructed by taking a line of initial conditions along the stable manifold of the linearized system and evolving them backward in time.

We can do better than this by choosing some parameter (like arclength) along the manifold and for each parameter decide how many iterations of the map would be required to take the point back to within some small region of the fixed point. We then choose an initial condition along the linearized eigenvectors and iterate the point back with the map. This idea is implemented in the following program:

```
(define ((unstable-manifold T xe ye dx dy A eps) param)
  (let ((n (floor->exact (/ (log (/ param eps)) (log A)))))
    ((iterated-map T n) (+ xe (* dx (/ param (expt A n))))
                        (+ ye (* dy (/ param (expt A n))))
                        cons
                        list)))
```

where `T` is the map, `xe` and `ye` are the coordinates of the fixed point, `dx` and `dy` are components of the linearized eigenvector, `A` is the characteristic multiplier, `eps` is a scale within which the linearized map is a good enough approximation to `T`, and `param` is a continuous parameter along the manifold. The program assumes that there is a basic exponential divergence along the manifold – that is why we take the logarithm of `param` to get initial conditions in the linear regime. This assumption is not exactly true, but good enough for now.

The curve is generated by a call to a `plot-parametric-fill`, which recursively subdivides intervals of the parameter until there are enough points to get a smooth curve.

```
(define (plot-parametric-fill win f a b near?)
  (let loop ((a a) (xa (f a)) (b b) (xb (f b)))
    (let ((m (/ (+ a b) 2)))
      (let ((xm (f m)))
        (plot-point win (car xm) (cdr xm))
        (if (not (and (near? xa xm) (near? xb xm)))
            (begin (loop a xa m xm)
                   (loop m xm b xb)))))))
```

The `near?` parameter is a test for whether two points are within a given distance of each other in the graph. Because some coordinates are angle variables, this may involve a principal value comparison. For example, for the driven pendulum section, the horizontal axis is an angle but the vertical axis is not, so the picture is on a cylinder:

```
(define (cylinder-near? eps)
  (let ((eps2 (square eps)))
    (lambda (x y)
      (< (+ (square ((principal-value pi)
                     (- (car x) (car y))))
            (square (- (cdr x) (cdr y))))
         eps2))))
```

Figure 4.9 shows a computation of the homoclinic tangle for the driven pendulum. The parameters are $m = 1kg$, $g = 9.8kgms^{-1}$, $l = 1m$, $\omega = 4.2\omega_0 = 4.2\sqrt{g/l}$, and amplitude $A = 0.05m$.

For reference Figure 4.10 shows a surface of section for these parameters on the same scale.

Exercise 4.6: Computing Homoclinic Tangles

a. Compute stable and unstable manifolds for the standard map.

b. Identify the features on the homoclinic tangle that entered the argument about its existence, such as the central crossing of the stable and unstable manifolds, etc.

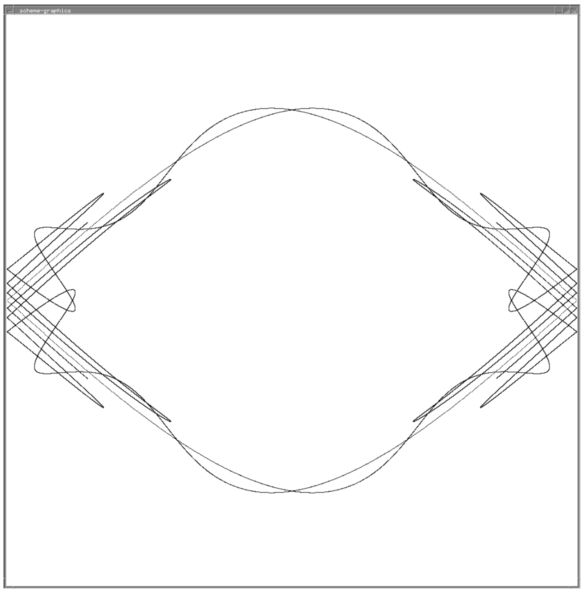

Figure 4.9 The computed homoclinic tangle for the driven pendulum exhibits the features described in the text. Notice how the excursions of the stable and unstable manifolds become longer and thinner as they approach the unstable fixed point.

c. Investigate the errors in the process. Are the computed manifolds really correct or a figment of wishful thinking? One could imagine that the errors are exponential and the computed manifolds have nothing to do with the actual manifolds.

d. How much actual space is taken up by the homoclinic tangle? Consider a value of the coupling constant $K = 0.8$. Does the homoclinic tangle actually fill out the apparent chaotic zone? Note: this is hard and we don't know the answer.

4.4 Integrable Systems

Islands appear near commensurabilities, and commensurabilities are present even in integrable systems. In integrable systems an infinite number of periodic orbits are associated with each commensurability, but upon perturbation only a finite number of periodic orbits survive. How does this happen? First we have to learn more about integrable systems.

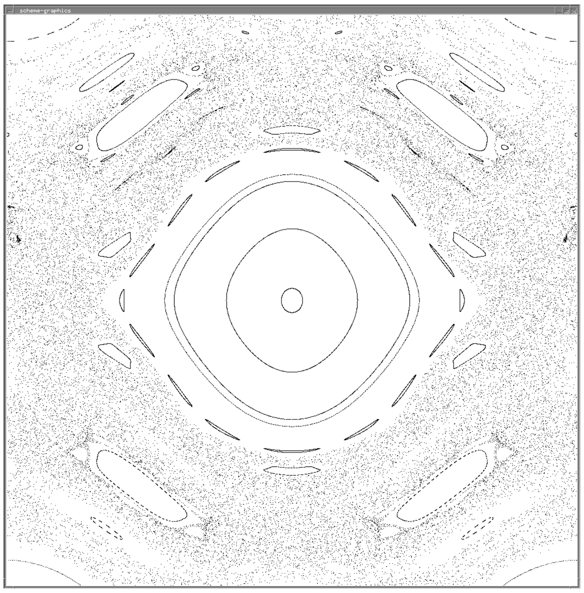

Figure 4.10 The section for driven pendulum with the same parameters as was used to construct the tangle. The tangle expands to fill space, occupying at least part of the chaotic region.

If an n degree of freedom system has n independent conserved quantities then the solution of the problem can be reduced to quadratures. Such a system is called *integrable*. Typically, the phase space of integrable systems is divided into regions of qualitatively different behavior. For example, the motion of a pendulum is reducible to quadratures, and has three distinct types of solutions: the oscillating solutions and the clockwise and counterclockwise circulating solutions. The different regions of the pendulum phase space are separated by the trajectories that are asymptotic to the unstable equilibrium. It turns out that for any system that is reducible to quadratures a set of phase space coordinates can be chosen for each region of the phase space so that the Hamiltonian describing the motion in that region depends only on the momenta. Furthermore if the phase space is bounded then the generalized coordinates can be chosen to be angles (that are 2π periodic). The configuration space described by n angles is an n-torus. The momenta conjugate to these angles are called *actions*. Such phase space coordinates are called *action-angle* coordinates. We will see how to reformulate systems in this way later. Here we explore the consequences of such a formulation; this formulation is especially useful for exploring what happens as additional effects are added to integrable problems.

Orbit Types in Integrable Systems

So suppose we have a time-independent n degree of freedom system that is reducible to quadratures. For each region of phase space there is a local formulation of the system so that the evolution of the system is described by a time-independent Hamiltonian that depends only on the momenta. Suppose further that the coordinates are all angles. Let θ be the tuple of angles, and J be the tuple of conjugate momenta. The Hamiltonian is

$$H(t, \theta, J) = H_0(J). \tag{4.35}$$

Hamilton's equations are simply

$$\begin{aligned} DJ(t) &= -\partial_1 H(t, \theta(t), J(t)) = 0 \\ D\theta(t) &= \partial_2 H(t, \theta(t), J(t)) = \omega(J(t)), \end{aligned} \tag{4.36}$$

where $\omega(J) = DH_0(J)$ is a tuple of frequencies with a component for each degree of freedom. The momenta are all constant because none of the coordinates appear in the Hamiltonian. The motion of the coordinate angles is uniform; the rate of change of the angles are the frequencies ω, which depend only on the constant momenta. Given inital values $\theta(t_0)$ and $J(t_0)$ at time t_0, the solutions are simple:

$$\begin{aligned} J(t) &= J(t_0) \\ \theta(t) &= \omega(J(t_0))(t - t_0) + \theta(t_0). \end{aligned} \tag{4.37}$$

If $\omega(J_0)$ is zero for some J_0 then $J = J_0$ is an equilibrium point of the system for any initial θ_0.

A solution is periodic if all the coordinates of the system return to the initial coordinates at some later time. Each coordinate θ_i with nonzero frequency $\omega_i(J_0)$ is periodic with a period $T_i = 2\pi/\omega_i(J_0)$. The period of the system T must therefore be an integer multiple k_i of each of the individual coordinate periods T_i: $T = k_i T_i$. If the system is periodic with some set of integer multiples, then it is also periodic with any common factors divided out. Thus the period of the system is $T = (k_i/d)T_i$ where d is the greatest common divisor of the integers k_i.

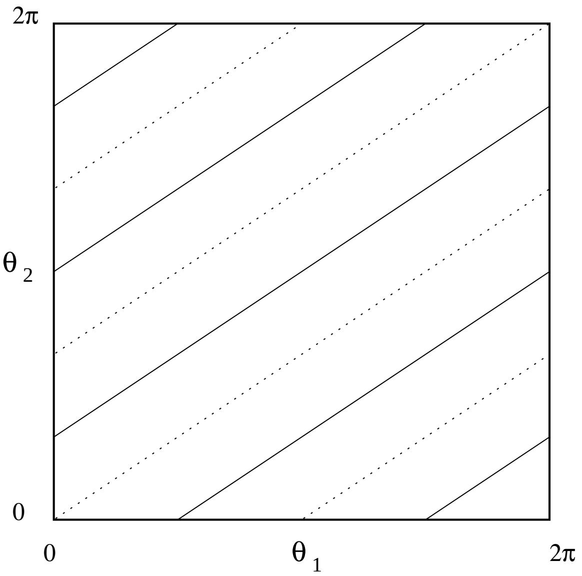

Figure 4.11 The solid and dotted lines show two periodic trajectories on the configuration coordinate plane. For commensurate coordinate frequencies the configuration motion is periodic, independent of the initial angles. In this illustration the frequencies satisfy $3\omega_1(J_0) = 2\omega_2(J_0)$. The rotation number is 2/3. The orbit closes after 3 cycles of θ_1 and 2 cycles of θ_2, for any initial θ_1 and θ_2.

For a system with two degrees of freedom a solution is periodic if there exist relatively prime integers k and j such that $k\omega_1 = j\omega_2$. The period of the system is $T = 2\pi j/\omega_1 = 2\pi k/\omega_2$; the frequency is $\omega_1/j = \omega_2/k$. A periodic motion on the 2-torus is illustrated in Figure 4.11.

In general, if the coordinate frequencies $\omega_i(J_0)$ satisfy an integer-coefficient relation $\sum_i n_i\omega_i = 0$ among its frequencies we say that the frequencies satisfy a commensurability. If there is no commensurability for any non-zero integer coefficients we say that the frequencies are linearly independent (with respect to the integers) and the solution is *quasiperiodic*. One can prove that for n incommensurate frequencies all solutions come arbitrarily close to every point in the configuration space.[5]

[5]Motion with n incommensurate frequencies is dense on the n-torus. Furthermore, such motion is *ergodic* on the n-torus. This means that time averages of

For a system with two degrees of freedom the solutions in a region described by a particular set of action-angle variables are either equilibrium solutions, periodic solutions, or quasiperiodic solutions.[6] For systems with more than two degrees of degrees of freedom there are trajectories that are neither periodic nor quasiperiodic with n frequencies. These are quasiperiodic with fewer frequencies and dense over a corresponding lower dimensional torus.

Surfaces of Section for Integrable Systems

As we have seen, in action-angle coordinates the angles move with constant angular frequencies, and the momenta are constant. Thus surfaces of section in action-angle coordinates are particularly simple. We can make surfaces of section for time-independent two degree of freedom systems or one degree of freedom systems with periodic drive. In the latter case, one of the angles in the action-angle system is the phase of the drive. We make surfaces of section by accumulating points in one pair of canonical coordinates as the other coordinate goes through some particular value, such as zero. If we plot the section points with the angle coordinate on the abscissa and the conjugate momentum on the ordinate then the section points for all trajectories lie on horizontal lines, as illustrated in figure 4.12.

For definiteness, let the plane of the surface of section be the (θ_1, J_1) plane, and the section condition be $\theta_2 = 0$. The other momentum J_2 is chosen so that all the trajectories have the same energy. The momenta are all constant, so for a given trajectory all points that are generated are constrained to a line of constant J_1.

The time between section points is the period of the θ_2: $\Delta t = 2\pi/\omega_2(J_0)$ because a section point is generated for every cycle of θ_2. The angle between successive points on the section is $\omega_1 \Delta t = \omega_1 2\pi/\omega_2 = 2\pi\nu$, where $\nu = \omega_1/\omega_2$ is called the *rotation number*

---

time independent phase space functions computed along trajectories are equal to the phase space average of the same function over the torus.

[6]For time-independent systems with two degrees of freedom the boundary between regions described by different action-angle coordinates has asymptotic solutions and unstable periodic orbits or equilibrium points. The solutions on the boundary are not described by the action-angle Hamiltonian.

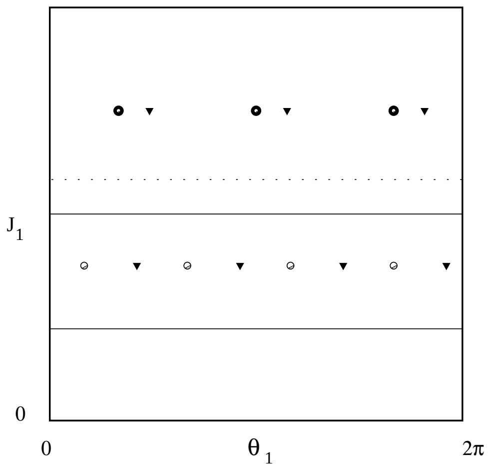

Figure 4.12 On surfaces of section for systems in action-angle coordinates all trajectories generate points on horizontal lines. Trajectories with frequencies that are commensurate with the sampling frequency produce a finite number of points. Trajectories with frequencies that are incommensurate with the sampling frequency fill out a horizontal line densely.

of the trajectory. Along a trajectory, the map from one section point $(\theta_1(i), J_1(i))$ to the next $(\theta_1(i+1), J_1(i+1))$ is of the form:

$$\begin{pmatrix} \theta_1(i+1) \\ J_1(i+1) \end{pmatrix} = T \begin{pmatrix} \theta_1(i) \\ J_1(i) \end{pmatrix} = \begin{pmatrix} \theta_1(i) + 2\pi\nu(J(i)) \\ J_1(i) \end{pmatrix} \tag{4.38}$$

If the rotation number is strictly monotonic in the action coordinate on the section then the map is called a *twist map*.[7]

On a surface of section the different types of orbits generate different patterns. If the orbit is an equilibrium solution then the initial point on the surface of section is a fixed point. The system just stays there.

If the two coordinate frequencies are commensurate then the trajectory is periodic and there are only a finite number of points generated on the surface of section. Both of the periodic solutions illustrated in Figure 4.11 generate two points on the surface of section defined by $\theta_2 = 0$. If the coordinate frequencies are com-

[7]Actually, to be a twist map we require $|D\nu(J)| > K > 0$ over some interval of J.

mensurate they satisfy a relation of the form $k\omega_1(J_0) = j\omega_2(J_0)$, where J_0 is the initial and constant value of the momentum tuple J. The frequency of the motion is $\omega_1/j = \omega_2/k$, so the period is $2\pi j/\omega_1 = 2\pi k/\omega_2$. Thus this periodic orbit generates k points on this surface of section. For trajectories with commensurate frequencies the rotation number is rational: $\nu = j/k$. The coordinate θ_2 makes k cycles while the coordinate θ_1 makes j cycles (Figure 4.11 shows a system with a rotation number of 2/3.). The frequencies depend on the momenta but not on the coordinates, so the motion is periodic with the same period and rotation number for all initial angles given these momenta. Thus there is a continuous family of periodic orbits with different initial angles.

If the two coordinate frequencies are incommensurate, then the 2-torus is filled densely. Thus the line on which the section points are generated is filled densely. Again, this is the case for any initial coordinates, because the frequencies depend only on the momenta. There are infinitely many such orbits which are distinct for a given set of frequencies.[8]

4.5 Poincaré-Birkhoff Theorem

How does this picture change if we add additional effects?

One peculiar feature of the orbits in integrable systems is that there are continuous families of periodic orbits. The initial angles do not matter, the frequencies depend only the actions. Contrast this with our earlier experience with surface of section in which periodic points are isolated, and associated with island chains. Here we investigate periodic orbits of near integrable systems, and find that typically for each rational rotation number there are a finite number of periodic points, half of which are linearly stable and half linearly unstable.

Consider an integrable system described in action-angle coordinates by the Hamiltonian $H_0(J)$. We add in some small additional effect described by the term H_1 in the Hamiltonian

$$H(t, \theta, J) = H_0(J) + \epsilon H_1(t, \theta, J). \tag{4.39}$$

[8] The section points for any particular orbit are countable and dense, but they have zero measure on the line.

An example of such a system is the periodically driven pendulum with small drive amplitude. For zero drive amplitude the driven pendulum is integrable, but not for small drive. Unfortunately, we do not yet have the tools to develop action-angle coordinates for the pendulum. A simpler problem that is already in action-angle form is the driven rotor, which is just the driven pendulum with gravity turned off. We can implement this by turning our driven pendulum on its side, making the plane of the pendulum horizontal. A Hamiltonian for the driven rotor is

$$H(t, \theta, p_\theta) = \frac{p_\theta^2}{2ml^2} + mlAw^2 \cos \omega t \cos \theta, \tag{4.40}$$

where A is the amplitude of the drive with frequency ω, m is the mass of the bob, and l is the length of the rotor. For zero amplitude, the Hamiltonian is already in action-angle form in that it depends only on the momentum p_θ and the coordinate is an angle.

For an integrable system, the map generated on the surface of section is of the form (4.38). With the additional of a small perturbation to the Hamiltonian, small corrections are added to the map

$$\begin{aligned}\begin{pmatrix} \theta_1(i+1) \\ J_1(i+1) \end{pmatrix} &= T_\epsilon \begin{pmatrix} \theta_1(i) \\ J_1(i) \end{pmatrix} \\ &= \begin{pmatrix} \theta_1(i) + 2\pi\nu(J(i)) + \epsilon f(\theta_1(i), J_1(i)) \\ J_1(i) + \epsilon g(\theta_1(i), J_1(i)) \end{pmatrix}. \end{aligned} \tag{4.41}$$

Both the map T and the perturbed map T_ϵ are area preserving because the maps are generated as surfaces of section for Hamiltonian systems.

Suppose we are interested in determining whether periodic orbits of a particular rational rotation number $\nu = j/k$ exist in some interval of the action $\alpha < J_1 < \beta$. If the rotation number is strictly monotonic in this interval and orbits with the rotation number ν occur in this interval for the unperturbed map T then by a simple construction we can show that periodic orbits with this rotation number also exist for T_ϵ for sufficiently small ϵ.

If a point is a periodic for rational rotation number $\nu = j/k$, with relatively prime j and k, we expect k distinct images of the point to appear on the section. So if we consider k^{th} iterate of the map then the point is a fixed point of the map. For rational

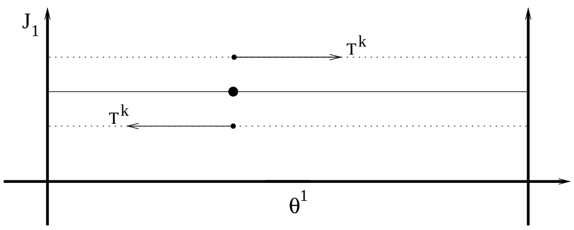

Figure 4.13 The map T^k has a line of fixed points if the rotation number is the rational j/k. Points above this line map to the larger θ_1; points below this line map to smaller θ_1

rotation number j/k the map T^k has a fixed point for every initial angle.

The rotation number of the map T is strictly monotonic. Suppose for definiteness we assume the rotation number $\nu(J_1)$ increases with J_1. For some J_1^* such that$\alpha < J_1^* < \beta$ the rotation number is j/k, and (θ_1, J_1^*) is a fixed point of T^k for any initial θ_1. For J_1^* the rotation number of T^k is zero. The rotation number of the map T is monotonically increasing so for $J_1 > J_1^*$ the rotation number of T^k is positive, and for $J_1 < J_1^*$ the rotation number of T^k is negative, as long as J_1 is not too far from J_1^*. See Figure 4.13.

Now consider the map T_ϵ^k. In general, for small ϵ, points map to slightly different points under T_ϵ than they do under T, but not too different. So we can expect that there is still some interval near J_1^* such that for J_1 in the upper end of the interval T_ϵ^k maps points to larger θ_1, and for points in the lower end of the interval maps decreases θ_1, as we saw for T^k. If this is the case then for every θ_1 there is a point somewhere in the interval, some J_1^+, for which θ_1 does not change, by continuity. These are not fixed points because the momentum J_1 generally changes. See Figure 4.14.

The map is continuous, so we can expect that J_1^+ is a continuous function of the θ_1. As we let θ_1 vary through 2π, either this function is periodic or not. That it must be periodic is a consequence of area preservation.[9] So the set of points that do not

[9]If J_1^+ were not periodic in θ_1 then it would have to spiral. Suppose it spirals. The region enclosed by two succesive turns of the spiral is mapped to a region between succesive turns of the spiral further down the spiral. The map preserves area, so the spiral cannot asymptote, but must progress infinitely down the cylinder. This is impossible because of the twist condition: sufficently far

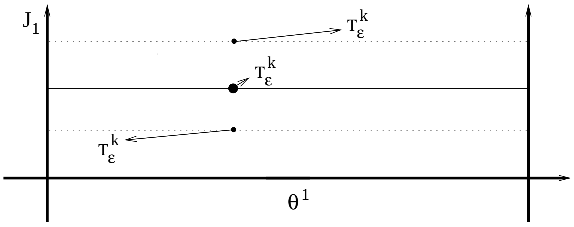

Figure 4.14 The map T_ϵ^k is slightly different from T^k, but above the central region points still map to larger θ_1 and below the central region they map to smaller θ_1. By continuity there are points between for which θ_1 does not change.

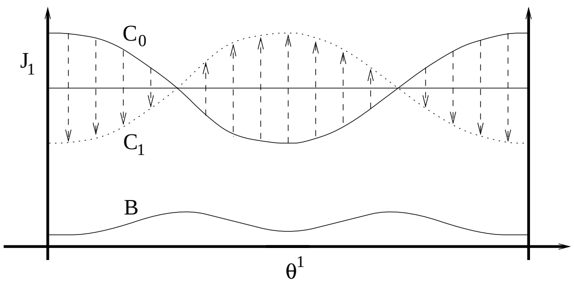

Figure 4.15 The curve C_0 of points that map to the same θ_1 under T_ϵ^k is indicated by the solid line. The image of this curve C_1 under T_ϵ^k is the dotted curve. Area preservation implies these curves cross.

change θ under T_ϵ^k form some periodic function of θ_1. Call this curve C_0. See Figure 4.15.

The map T_ϵ^k takes the curve C_0 to another curve C_1, which, like C_0, is continuous and periodic. The two curves C_0 and C_1 must cross each other, as a consequence of area preservation. How do we see this? Typically, there is a lower boundary or upper boundary for the evolution J_1. In some situations, we have such a lower boundary because J_1 cannot be negative. For example, in action-angle variables for motion near a elliptic fixed point we will see that the action is the area enclosed on the phase plane, which cannot be negative. For others, we might use the fact that there are invariant curves for large positive or negative J_1. In any

down the cylinder the rotation number is too different to allow the angle to be the same under T_ϵ^k. So J_1^+ does not spiral.

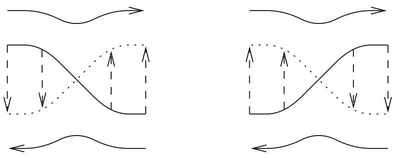

Figure 4.16 The fixed point on the left is linearly unstable. The one on the right is linearly stable.

case, suppose there is such a barrier B. Then, the area of the region between the barrier and C_0 must be equal to the area of the image of this region, which is the region between the barrier and the curve C_1. So if at any point the two curves C_0 and C_1 do not coincide, then they must cross to contain the same area. In fact, they must cross an even number of times because they are both periodic so if they cross once they must cross again to get back to the same side they started on. The points at which the curves C_0 and C_1 cross are fixed points because the angle does not change (that is what it means to be on C_0) and the action does not change (that is what it means for C_0 and C_1 to be the same at this point). So we have deduced that there must be an even number of fixed points of T_ϵ^k. For each fixed point of T_ϵ^k there are k images of this fixed point under T_ϵ on the surface of section.

We can deduce the stability of these fixed points just from the construction. The fixed points come in two types, elliptic and hyperbolic. A elliptic fixed point appears where the flow is around the fixed point: the map from C_0 to C_1 can be continued along the background flow to make a closed curve. A hyperbolic fixed point appears where if we follow the map from C_0 to C_1 we enter the background flow in such a way as to leave the fixed point. So just from the way the arrows connect we can determine the character of the fixed point. See Figure 4.16.

As we develop a Poincaré section, we find that some orbits leave traces that circulate around the stable fixed points, resulting in the Poincaré-Birkhoff islands. If we look at a particular island we see that orbits in the island circulate around the fixed point at a rate that is monotonically dependent upon the distance from the fixed point. In the vicinity of the fixed point the evolution is governed by a twist map. So the entire Poincaré-Birkhoff construction can be carried out again. We expect that there will be concentric families of stable periodic points surrounded by islands and separated by separatrices emanating from unstable periodic points. Around each of these stable periodic orbits, the construction is repeated. So the Poincaré-Birkhoff construction is recursive, leading to the development of an infinite hierarchy of structure.

Computing the Poincaré-Birkhoff Construction

There are so many conditions in our construction of the fixed points that one might be suspicious. We can make the construction more convincing by actually computing the various pieces for a specific problem. Consider the periodically driven rotor, with Hamiltonian (4.40). We set $m = 1kg$, $l = 1m$, $A = 0.1m$, $\omega = 4.2\sqrt{9.8}$.

We call points that map to the same angle "radially mapping points." We find them with a simple bisection:

```
(define (radially-mapping-points map Jmin Jmax phi eps)
  (bisect
    (lambda (J)
      ((principal-value pi)
       (- phi (map phi J (lambda (phip Jp) phip) list))))
    Jmin Jmax eps))
```

We provide procedure `map` implementing some map, which may be an iterate of some more primitive map. We give the procedure an angle `phi` to study and a range of actions `Jmin` to `Jmax` to search, and a tolerance `eps` for the solution.

We make a plot of the curves C_0 (of initial conditions that map radially) and C_1 (the image of C_0) with an appropriate piece of wrapper code.

In Figure 4.17 we show the Poincaré-Birkhoff construction of the fixed points for the driven rotor. These particular curves are constructed for the two 1:1 commensurabilities between the rotation and the drive. There is one set of fixed points constructed for each sense of rotation. The corresponding section is in Figure 4.18. We see that the section shows the existence of fixed points exactly where the Poincaré-Birkhoff construction shows the crossing of the curves C_0 and C_1. Indeed, we can see that the nature of the fixed point is clearly reflected in the relative configuration of the C_0 and C_1 curves.

In Figure 4.19 we show the result for a rotation number of 1/3. The curves are the radially mapping points for the third iterate of the section map (solid) and the images of these points (dotted). These curves are distorted by their proximity to the 1:1

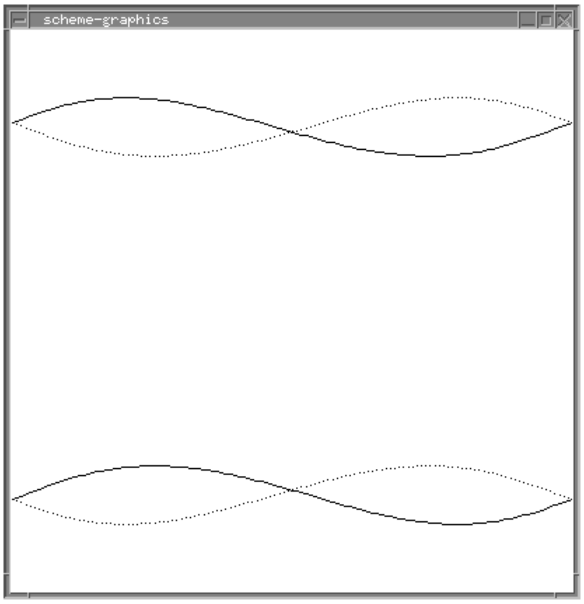

Figure 4.17 The curves C_0 (solid) and C_1 (dotted) for the 1:1 commensurability. The angle runs from $-\pi$ to π. The momentum runs from -20 to 20 in appropriate units.

islands shown in Figure 4.18. The corresponding section is shown in Figure 4.20.

4.6 Invariant Curves

We started with an integrable system, where there are invariant curves.

The Poincaré-Birkhoff construction for twist maps shows that invariant curves with rational rotation number typically do not survive perturbation. Upon perturbation the invariant curves with rational rotation numbers are replaced by an alternating sequence of stable and unstable periodic orbits. So if there are invariant curves that survive perturbation they must have irrational rotation numbers.

When we added a perturbation, we got chains of alternating stable and unstable fixed points for every rational rotation number, and each stable fixed point is surrounded by an island. Since the rational numbers are dense one might wonder if any invariant

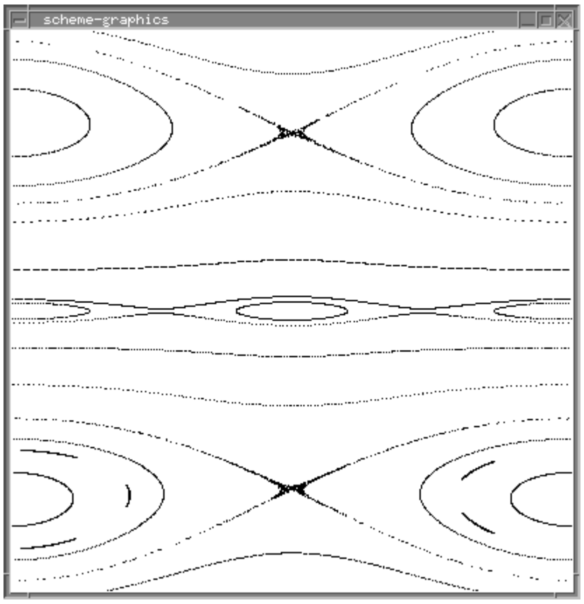

Figure 4.18 The surface of section displaying the 1:1 commensurability. The angle runs from $-\pi$ to π. The momentum runs from -20 to 20 in appropriate units.

curve survives the perturbation. Surely there are even more irrational rotation numbers to look at, but each irrational is arbitrarily close to a rational, so it is not obvious that any invariant curve survives an arbitrarily small perturbation. The Kolomogorov-Arnold-Moser (KAM) theorem proves invariant curves exist if the perturbation is small enough, so that the perturbed problem is "close enough" to an integrable problem, and if the rotation number is "irrational enough." We will not prove this theorem here. Instead we will develop methods for finding particular invariant curves.

Stable periodic orbits have a stable island surrounding them on the surface of section. The largest islands are associated with rationals with small denominators. In general the size of the island is limited to a size that decreases as the denominator increases. These islands are a local indication of the effect of the perturbation. Similarly, the chaotic zones appear near unstable periodic orbits and their homoclinic tangles. The homoclinic tangle is a continuous curve so it cannot cross an invariant curve, which is

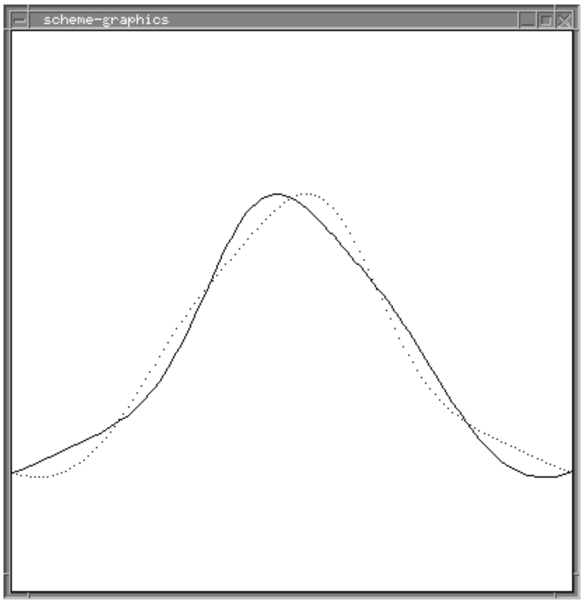

Figure 4.19 The curves C_0 (solid) and C_1 (dotted) for the 1:3 commensurability. The angle runs from $-\pi$ to π. The momentum runs from 3.5 to 4.5 in appropriate units.

also continuous. If we are looking for invariant curves that persist upon perturbation, we would be wise to avoid regions of phase space where the islands or homoclinic tangles are major features.

The Poincaré-Birkhoff islands are ordered by rotation number. Because of the twist condition, the rotation number is monotonic in the momentum of the unperturbed problem. If there is an invariant curve with a given rotation number it is sandwiched between island chains associated with rational rotation numbers. The rotation number of the invariant curve must be between the rotation numbers of the island chains on either side of it.

The fact that the size of the islands descreases with the size of the denominator suggests that invariant curves with rotation numbers for which nearby rationals require large denominators are the most likely to exist. So we will begin our search for invariant curves by examining rotation numbers that are not near rationals with small denominators.

Any irrational can be approximated by a sequence of rationals, and for each of these rationals we expect there to be stable and

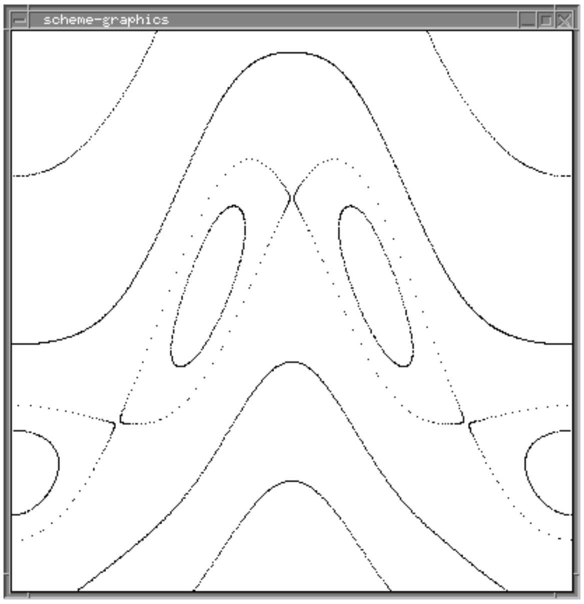

Figure 4.20 The surface of section displaying the 1:3 commensurability. The angle runs from $-\pi$ to π. The momentum runs from 3.5 to 4.5 in appropriate units.

unstable periodic orbits with stable islands and homoclinic tangles. An invariant curve for a given rotation number has the best chance of surviving if the size of the islands associated with the each rational approximation is smaller than the separation of the islands from the invariant curve with that rotation number.

For any particular size deonminator, the best rational approximation to an irrational number is given by an initial segment of a simple continued fraction. If the approximating continued fraction converges slowly to the irrational number then that number is not near rationals with small denominators. Thus, we will look for invariant curves with rotation numbers that have slowly converging continued-fraction approximations. The continued fractions that converge most slowly have tails that are all one. For example, the golden ratio,

$$\phi = \frac{1+\sqrt{5}}{2} = 1 + \frac{1}{1+\frac{1}{1+\frac{1}{1+\cdots}}}, \tag{4.42}$$

is just such a number.

Finding Invariant Curves

Invariant curves, if there are any, are characterized by a particular rotation number. Points on the invariant curve map to points on the invariant curve. Neighboring points map to neighboring points, preserving the order.

On the section for the unperturbed integrable system, the angle between successive section points is constant: $\Delta\theta = 2\pi\nu$, for rotation number ν. This map of the circle onto itself with constant angular step we call a uniform circle map.

For a given rotation number points on the section are laid down in a particular order characteristic of the rotation number only. As a perturbation is turned on, the invariant curve with a particular rotation number will be distorted and the angle between successive points will no longer be constant. All that is required to have a particular rotation number is that the average change in angle is $\Delta\theta$. Nevertheless, the ordering of the points on the surface of section is preserved, and is characteristic of the rotation number.

We can use the fact that the sequence of points on the surface of section for an invariant curve with a given rotation number must have a particular order to find the invariant curve. By evolving a candidate initial point with both the perturbed map and the uniform circle map and comparing the ordering of the sequence of points that are generated we can tell whether the initial point is on the desired invariant curve or to which side it is.

Suppose we have a map that we can iterate to get the points on a section. Using the idea of comparing the ordering of points with the ordering of the uniform circle map, to indicate how the rotation number of our orbit compares to the specified, we can find the momentum for the invariant curve by bisection search:[10]

```
(define (find-invariant-curve map rn theta0 Jmin Jmax eps)
  (bisect (lambda (J) (which-way? rn theta0 J map))
          Jmin Jmax eps))
```

However, we need to be able to determine which way to change the momentum to approach the required rotation number.

[10]This depends on the assumptions that `Jmin` and `Jmax` bracket the actual momentum, and that the rotation number is sufficiently continuous in momentum in that region.

We can evolve the orbits for both maps, producing streams of points that appear on the section. (The momentum value of the uniform circle map is superfluous.) Each orbit stream is transduced into a stream of positive integers. The integers give the number of points that have been examined in the stream that have smaller values of the angle. The streams of integers are then compared until a discrepancy is found. The first discrepancy is used to compare the rotation numbers of the two orbits, to determine which orbit has smaller rotation number.

```
(define (which-way? rn theta0 J0 map)
  (compare-streams
   (position-stream theta0
                    (orbit-stream map theta0 J0)
                    '())
   (position-stream theta0
                    (orbit-stream (uniform-circle-map rn) theta0 J0)
                    '())
   0))
```

The maps are evolved and built into a stream by a simple recursive procedure. The maps are represented in the same way that they appeared in section 3.6.

```
(define (orbit-stream the-map x y)
  (cons-stream (list x y)
               (the-map x y
                        (lambda (nx ny)
                          (orbit-stream the-map nx ny))
                        (lambda () 'fail))))
```

The `uniform-circle-map` is a simple map that has a uniformly progressing angle with constant momentum.

```
(define (uniform-circle-map rotation-number)
  (let ((delta-theta (* :2pi rotation-number)))
    (lambda (theta y result fail)
      (result ((principal-value :2pi) (+ theta delta-theta))
              y))))
```

The procedure `position-stream` produces a stream of index positions. It maintains an ordered list of angle values, and as each new angle is added to the list it adds the position index to the stream. A principal value is applied to the angle to bring it to a uniform range specified.

```
(define (position-stream cut orbit list)
  (insert! ((principal-value cut) (car (head orbit)))
           list
           (lambda (nlist position)
             (cons-stream
               position
               (position-stream cut (tail orbit) nlist)))))
```

Given a new element `x` to be inserted into an ordered set `set` the procedure `insert!` calls its continuation with the updated set and the index that was used to insert the new element.[11]

The streams of indices are compared with `compare streams`. The count is used to keep track of how many points we have already entered into the circle. When there is a discrepancy between the indices, it means that one stream has begun to lead the other. The `principal-range` procedure is used to determine which is the leader.[12] This is analogous to using the principal value to determine the direction from one angle to another on a circle.

```
(define (compare-streams s1 s2 count)
  (if (= (head s1) (head s2))
      (compare-streams (tail s1) (tail s2) (+ count 1))
      ((principal-range count) (- (head s2) (head s1)))))
```

---

[11] The insert procedure is ugly:

```
(define (insert! x set cont)
  (cond ((null? set)
         (cont (list x) 1))
        ((< x (car set))
         (cont (cons x set) 0))
        (else
         (let lp ((i 1) (lst set))
           (cond ((null? (cdr lst))
                  (set-cdr! lst (cons x (cdr lst)))
                  (cont set i))
                 ((< x (cadr lst))
                  (set-cdr! lst (cons x (cdr lst)))
                  (cont set i))
                 (else
                  (lp (+ i 1) (cdr lst))))))))
```

[12] The `principal-range` procedure is implemented as follows:

```
(define ((principal-range period) index)
  (let ((t (- index (* period (floor (/ index period))))))
    (if (< t (/ period 2.))
        t
        (- t period))))
```

Once we have created this mess we can use it to find the initial momentum (for a given initial angle) for an invariant curve with a given rotation number. We search the standard map for an invariant curve with a golden rotation number:[13]

```
(find-invariant-curve (standard-map 0.95)
                      (- 1 (/ 1 golden-mean))
                      0.0
                      2.0
                      2.2
                      1e-5)
;Value: 2.114462280273437
```

This algorithm, although correct, has terrible performance. The problem is that each orbit builds a table of length the number of points examined, and each insertion of a new point scans that table sequentially, thus making a process that grows as the square of the number of points examined in time and as the number of points examined in space.

However, we observe that as ordering inconsistencies are found the angle are usually near the initial angle. We can make use of this to simplify the algorithm. Instead of keeping track of the whole list of angles, we can keep track of a small list of angles near the initial angle. In fact, keeping track of the nearest angle on either side of the initial angle works well. Here is the complete replacement for the `which-way?` procedure and its helpers. The procedure is implemented as a simple loop with state variables for the two orbits and the endpoints of the intervals. The `z` variables keep track of the angle of the uniform circle map; the `x` variables keep track of the angle of the map under study. The `y` variable is the momentum for the map under study. On each iteration the we determine if the angle of the uniform circle map is in the interval of interest below or above the initial angle. If it is in neither interval then the map is further iterated. However, if it is in the region of interest then we check to see if the angle of the other map is in the corresponding interval. If so, the intervals for the uniform circle map and the other map are narrowed and the iteration proceeds. If the angle is not in the required interval, a

[13] There is no invariant curve in the standard map with rotation number $\phi = 1.618\ldots$. However $1 - 1/\phi$ has the same continued-fraction tail as ϕ and there are rotation numbers of this size in the standard map.

discrepancy is noted and the sign of the discrepancy is reported. For this process to make sense the differences between the angles for successive iterations of both maps must be less than π.

```
(define (which-way? rotation-number x0 y0 the-map)
  (let ((pv (principal-value (+ x0 pi))))
    (let lp ((z x0) (zmin (- x0 :2pi)) (zmax (+ x0 :2pi))
             (x x0) (xmin (- x0 :2pi)) (xmax (+ x0 :2pi))
             (y y0))
      (let ((nz (pv (+ z (* :2pi rotation-number)))))
        (the-map x y
             (lambda (nx ny)
               (let ((nx (pv nx)))
                 (cond ((< x0 z zmax)
                        (if (< x0 x xmax)
                            (lp nz zmin z nx xmin x ny)
                            (if (> x xmax) 1 -1)))
                       ((< zmin z x0)
                        (if (< xmin x x0)
                            (lp nz z zmax nx x xmax ny)
                            (if (< x xmin) -1 1)))
                       (else
                        (lp nz zmin zmax nx xmin xmax ny)))))
             (lambda ()
               (error "Map failed" x y)))))))
```

With this method of comparing rotation numbers we can expect to be able to find the initial conditions for an invariant curve to high precision:

```
(find-invariant-curve (standard-map 0.95)
                      (- 1 (/ 1 golden-mean))
                      0.0
                      2.0
                      2.2
                      1e-16)
;Value: 2.1144605494391726
```

Using initial conditions computed in this way we can produce the invariant curve. See figure 4.21. If we expand the putative invariant curve it should remain a curve for all mangnifications—it should show no sign of chaotic fuzziness. See figure 4.22.

As can be seen from figure 4.22 the points on an invariant curve are not uniformly visited, unlike the picture we would get plotting the angles for the uniform circle map. This is because an interval may be expanded or compressed when mapped. We can compute

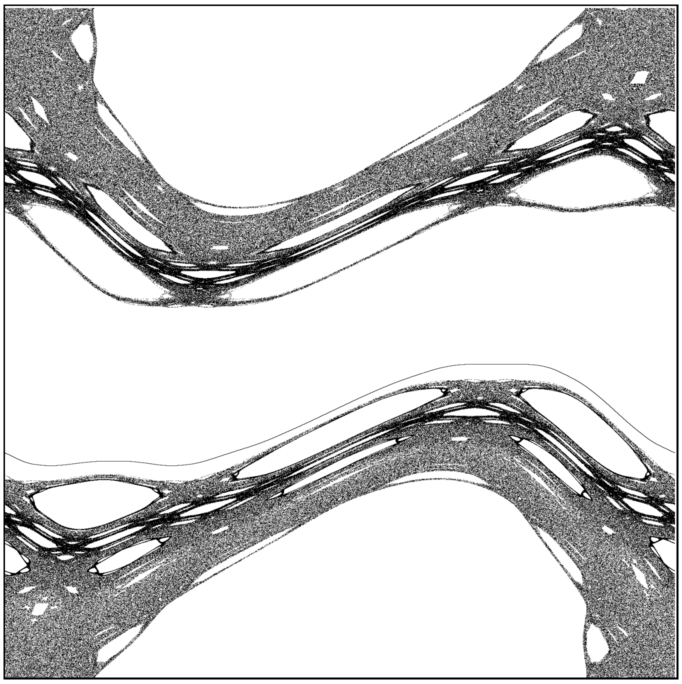

Figure 4.21 The surface of section displaying the invariant curve at rotation number $1 - 1/\phi$ for the standard map with $K = .95$. The invariant curve is in context: there is a chaotic region that almost eats the curve. The angle and momentum run from 0 to 2π.

the relative probability density for visitation of each angle on the invariant curve. A crude way to obtain this result is to count the number of points that fall into equal incremental angle bins. It is more effective to use the linear variational map constructed from the map being investigated to allow us to compute the change in incremental angle from one point to its successor. Since all of the points in a small interval around the source point are mapped to points (in the same order) in a small interval around the target point, the relative probability density at a point is inversely proportional to the size of the incremental interval around that point. In order to get this started we need a good estimate of the initial slope for the invariant curve. We can estimate the slope by a difference quotient of the momentum and angle increments for the interval that we used to refine the momentum of the invariant curve with a given rotation number. Figures 4.23, 4.24 and 4.25

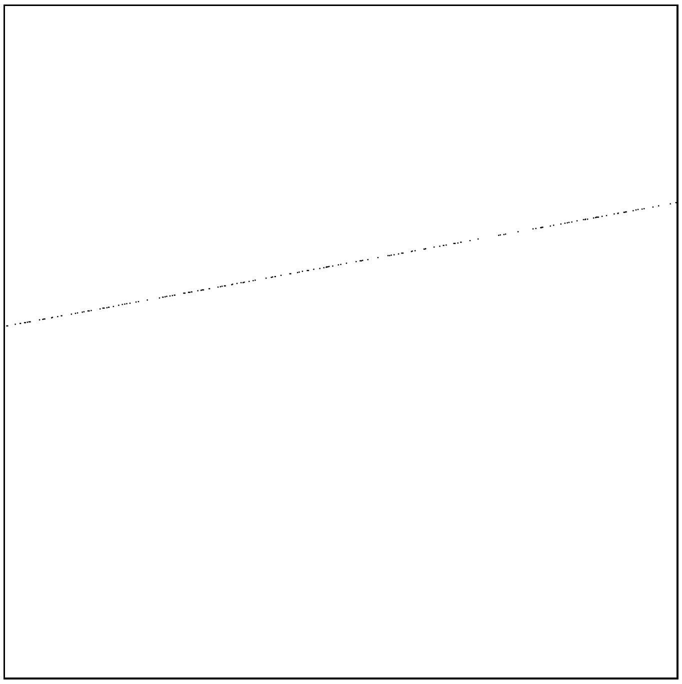

Figure 4.22 Here is a small portion of the same invariant curve shown in figure 4.21. The curve is magnified by $2 \times 10^7\pi$. We see that even at this magnification the points appear to lie on a line. We also see that the visitation frequency of points is highly nonuniform.

show the relative probability density of visitation as a function of angle for the invariant curve of golden winding number in the standard map for three different values of the parameter K. As K increases, certain angles become less likely. Near $K = 0.971635406$ some angles are never visited. But the invariant curve must be continuous. Thus it appears that for larger K the invariant curve with this rotation number will not exist. Indeed, if the invariant set persists with the given rotation number it will have an infinite number of holes (because it has an irrational winding number). Such a set is sometimes called a *cantorus*.

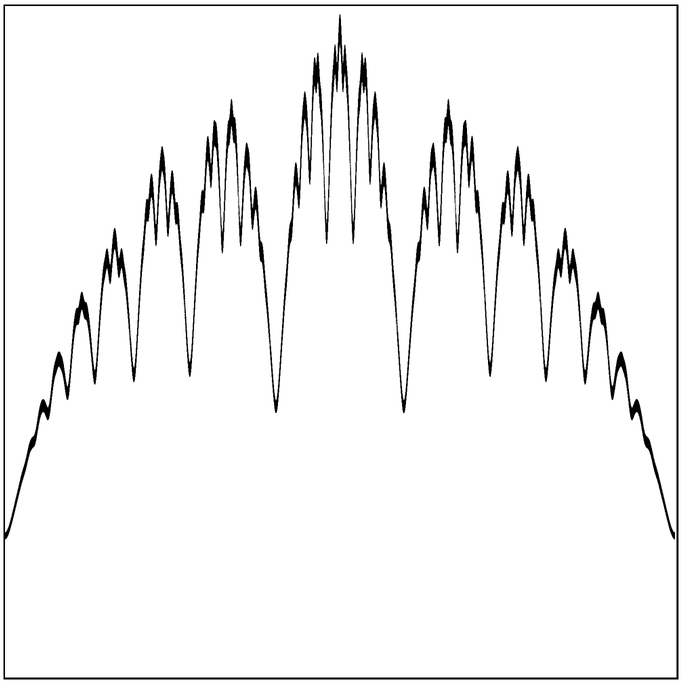

Figure 4.23 The relative probability density of visitation as a function of angle for the invariant curve of golden winding number in the standard map with $K = 0.95$.

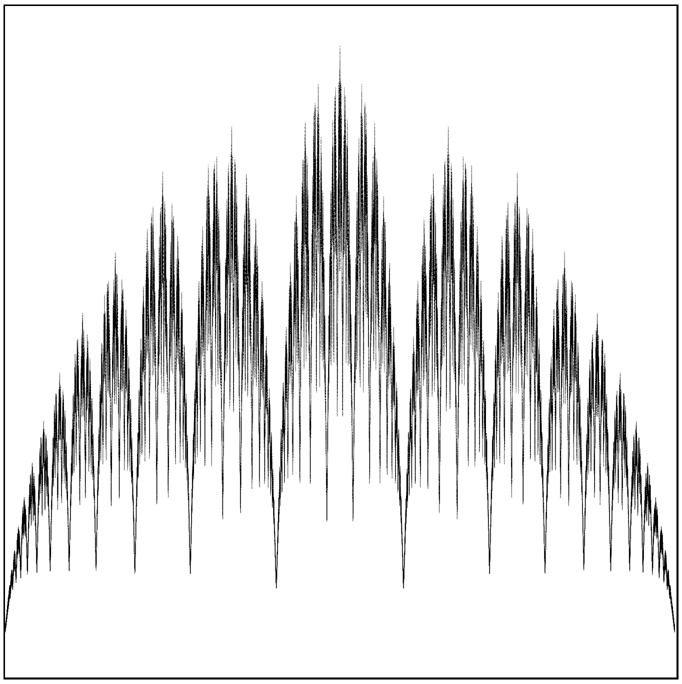

Figure 4.24 The relative probability density of visitation as a function of angle for the invariant curve of golden winding number in the standard map with $K = 0.97$. When compared with the corresponding plot for $K = 0.95$ the function has increased in complexity: there are more peaks and valleys. The valleys are deeper, indicating that there are angles that have become less likely to be visited.

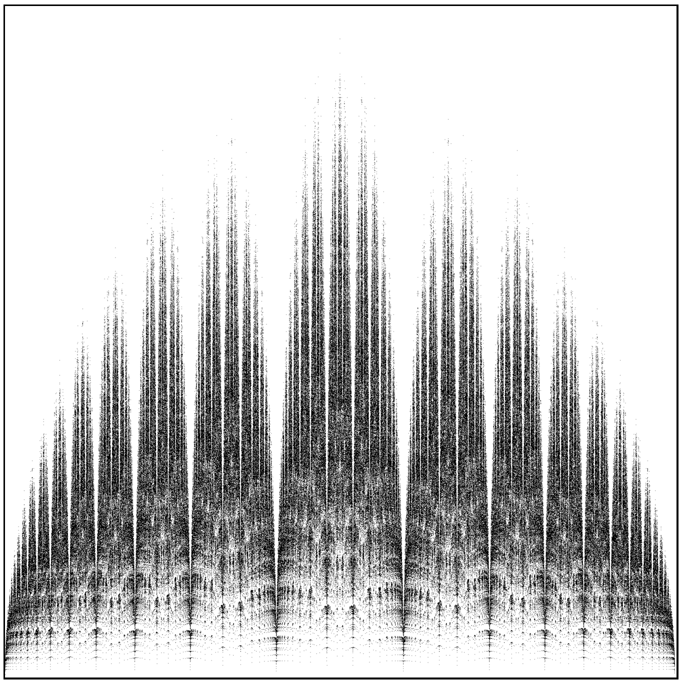

Figure 4.25 The relative probability density of visitation as a function of angle for the invariant curve of golden winding number in the standard map with $K = 0.971635406$. Here the function is very complex and appears self similar. The valleys appear to reach to zero, so there are discrete angles that are never visited.

5
Canonical Transformations

One way to simplify the analysis of a problem is to express the problem in a form where the solution has a simple representation. However, the initial formulation of the problem may be easier to express in other terms. For example, the formulation of the problem of the motion of a number of gravitating bodies is simple in rectangular coordinates, but it is easier to understand aspects of the motion in terms of orbital elements, such as the semimajor axes, eccentricities, and inclinations of the orbits. This transformation simplifies the problem of motion in a central potential. The semimajor axis and eccentricity of an orbit depend on both the configuration and the velocity of the body. So we need transformations that are more general than those that express changes in configuration coordinates. Here we investigate transformations of phase space coordinates that involve both the generalized coordinates and the generalized momenta.

A *canonical transformation* is a phase space coordinate transformation and an associated transformation of the Hamiltonian such that the dynamics given by Hamilton's equations in the two representations describe the same evolution of the system.

What transformations of phase space coordinates are allowed? How do we tell if a given reformulation of a problem describes the same motion? How do we construct transformations that are useful in the solution of a particular problem?

5.1 Point Transformations

A *point transformation* is a canonical transformation that extends a possibly time-dependent transformation of the configuration coordinates to a phase space transformation. For example, one might want to reexpress motion in terms of polar coordinates, given a description in terms of rectangular coordinates. In order to extend a transformation of the configuration coordinates to a phase space transformation we must specify how the momenta and Hamiltonian are transformed.

We have already seen how configuration transformations can be carried out in the Lagrangian formulation. In that case, we found that if the Lagrangian transforms by composition with the coordinate transformation, then the Lagrange equations are equivalent.

Lagrangians that differ by the addition of a total time derivative are equivalent, but have different momenta conjugate to the generalized coordinates. So there is more than one way to make a canonical extension of a coordinate transformation.

Here, we find that particular canonical extension of a coordinate transformation for which the Lagrangians transform by composition with the transformation, with no extra total time derivative terms added to the Lagrangian.

Let L be a Lagrangian for a system. Consider the coordinate transformation $q = F(t, q')$. From section 1.6.1, the velocities transform by

$$v = \partial_0 F(t, q') + \partial_1 F(t, q')v'. \tag{5.1}$$

We can obtain a Lagrangian in the transformed coordinates by composition $L'(t, q', v') = L(t, q, v)$

$$L'(t, q', v') = L(t, F(t, q'), \partial_0 F(t, q') + \partial_1 F(t, q')v'). \tag{5.2}$$

The momentum conjugate to q' is

$$\begin{aligned} p' &= \partial_2 L'(t, q', v') \\ &= \partial_2 L(t, F(t, q'), \partial_0 F(t, q') + \partial_1 F(t, q')v')\, \partial_1 F(t, q') \\ &= p\partial_1 F(t, q'), \end{aligned} \tag{5.3}$$

where we have used

$$\begin{aligned} p &= \partial_2 L(t, q, v) \\ &= \partial_2 L(t, F(t, q'), \partial_0 F(t, q') + \partial_1 F(t, q')v'). \end{aligned} \tag{5.4}$$

So, from equation (5.3),[1]

$$p = p'(\partial_1 F(t, q'))^{-1}. \tag{5.5}$$

We can collect these results to define a canonical phase space transformation C:[2]

$$\begin{aligned}(t, q, p) &= C(t, q', p') \\ &= (t, F(t, q'), p'(\partial_1 F(t, q'))^{-1}).\end{aligned} \tag{5.6}$$

The Hamiltonian is obtained by the Legendre transform

$$\begin{aligned}H'(t, q', p') &= p'v' - L'(t, q', v') \\ &= (p\partial_1 F(t, q'))\left((\partial_1 F(t, q')^{-1}(v - \partial_0 F(t, q')))\right) \\ &\quad - L(t, q, v) \\ &= pv - p\partial_0 F(t, q') - L(t, q, v) \\ &= H(t, q, p) - p\partial_0 F(t, q'),\end{aligned} \tag{5.7}$$

using relations (5.1) and (5.5) in the second step. Fully expressed in terms of the transformed coordinates and momenta the transformed Hamiltonian is

$$\begin{aligned}H'(t, q', p') &= H(t, F(t, q'), p'(\partial_1 F(t, q'))^{-1}) \\ &\quad - (p'(\partial_1 F(t, q'))^{-1})\partial_0 F(t, q').\end{aligned} \tag{5.8}$$

The Hamiltonians H' and H are equivalent because L and L' have the same value for a given dynamical state and so have the same paths of stationary action. In general H and H' do not have the same values for a given dynamical state, but differ by a term that depends on the coordinate transformation.

---

[1] Solving for p in terms of p' involves multiplying equation (5.3) on the right by $(\partial_1 F(t, q'))^{-1}$. This inverse is the structure that when multiplying $\partial_1 F(t, q')$ on the right gives a identity structure. Structures representing linear transformations may be represented in terms of matrices. In this case, the matrix representation of the inverse structure is the inverse matrix of the matrix representing the given structure.

[2] In chapter 1 the transformation C takes a local tuple in one coordinate system and gives a local tuple in another coordinate system. In this chapter C is a phase-space transformation.

For time-independent transformations, $\partial_0 F = 0$, there are a number of simplifications. The relationship of the velocities (5.1) becomes

$$v = \partial_1 F(t, q')v'. \tag{5.9}$$

Comparing this to the relation (5.5) between the momenta, we see that in this case the momenta transform "oppositely" to the velocity[3]

$$pv = p'(\partial_1 F(t, q'))^{-1}\partial_1 F(t, q')v' = p'v', \tag{5.10}$$

so the product of the momenta and the velocities is not changed by the transformation. This, combined with the fact that by construction $L(t, q, v) = L'(t, q', v')$, shows that, for this case, the Hamiltonian transforms by composition

$$\begin{aligned} H(t, q, p) &= pv - L(t, q, v) \\ &= p'v' - L'(t, q', v') \\ &= H'(t, q', p'). \end{aligned} \tag{5.11}$$

We can also see this from the general relationship (5.8) between the Hamiltonians.

Implementing Point Transformations

The procedure `F->CT` takes a procedure implementing a transformation of configuration coordinates `F` and returns a procedure implementing a transformation of phase-space coordinates.

```
(define ((F->CT F) H-state)
  (let ((t (time H-state))
        (q (coordinate H-state))
        (p (momentum H-state)))
    (->H-state t
               (F t q)
               (* p (invert (((partial 1) F) t q))))))
```

[3]The velocities and the momenta are dual geometric objects with respect to time-independent point transformations. The velocities comprise a vector field on the configuration manifold, and the momenta comprise a covector field on the configuration manifold. The invariance of the inner product pv under point transformations provides the motivation for the use of superscripts for velocity components and subscripts for momentum components in our notation.

For example, as previously noted, polar coordinates are often helpful in systems with radial symmetry. Consider a particle moving in a central field. In rectangular coordinates a Hamiltonian is:

```
(define ((H-central m V) H-state)
  (let ((x (coordinate H-state))
        (p (momentum H-state)))
    (+ (/ (square p) (* 2 m))
       (V (sqrt (square x))))))
```

Let's look at this Hamiltonian in polar coordinates. The transformation is time-independent so the Hamiltonian transforms by composition. The phase space transformation is obtained by applying `F->CT` to the procedure `p->r` that takes a time and a polar tuple and returns a tuple of rectangular coordinates (see section 1.6.1). In polar coordinates the Hamiltonian is:

```
(show-expression
 ((compose (H-central 'm (literal-function 'V))
           (F->CT p->r))
  (->H-state 't
             (coordinate-tuple 'r 'phi)
             (momentum-tuple 'p_r 'p_phi))))
```

$$\boxed{V(r) + \frac{\frac{1}{2}p_r^2}{m} + \frac{\frac{1}{2}p_\phi^2}{mr^2}}$$

There are three terms. There is the potential energy, which depends on the radius, there is the kinetic energy due to radial motion, and there is the kinetic energy due to tangential motion. As expected, the angle ϕ does not appear and thus the angular momentum is a conserved quantity. By going to polar coordinates we have decoupled one of the two degrees of freedom in the problem.

Exercise 5.1: Rotations

Let q and q' be rectangular coordinates that are related by a rotation R: $q = Rq'$. The Lagrangian for the system is $L(t, q, v) = \frac{1}{2}mv^2 - V(q)$. Find the corresponding phase space tranformation C. Do the momenta rotate with the coordinates?

5.2 General Canonical Transformations

Although we have shown how to extend any point transformation of the configuration space to a canonical transformation, there are other ways to construct canonical transformations. How do we know if we have a canonical transformation? To test if a transformation is canonical we may use the fact that if the transformation is canonical then Hamilton's equations of motion for the transformed system and the original system will be equivalent.

Consider a Hamiltonian H and a phase space transformation C. The transformation C transforms the phase space path $\sigma'(t) = (t, q'(t), p'(t))$ into $\sigma(t) = (t, q(t), p(t))$:

$$\sigma = C \circ \sigma'. \tag{5.12}$$

The rates of change of the phase-space coordinates are transformed by the derivative of the transformation

$$D\sigma = D(C \circ \sigma') = (DC \circ \sigma')D\sigma'. \tag{5.13}$$

Let D_s be the phase-space derivative operator

$$D_s H(t, q, p) = (1, \partial_2 H(t, q, p), -\partial_1 H(t, q, p)) . \tag{5.14}$$

Hamilton's equations are

$$D\sigma = D_s H \circ \sigma, \tag{5.15}$$

for any realizable phase-space path σ.

The transformation is canonical if the equations of motion obtained from the new Hamiltonian are the same as those that could be obtained by transforming the equations of motion derived from the original Hamiltonian to the new coordinates:

$$D\sigma = (DC \circ \sigma')D\sigma' = (DC \circ \sigma')D_s H' \circ \sigma' \tag{5.16}$$

Comparing equation (5.15) with this we see

$$D_s H \circ \sigma = (DC \circ \sigma')D_s H' \circ \sigma'. \tag{5.17}$$

Using $\sigma = C \circ \sigma'$ we find

$$D_s H \circ C \circ \sigma' = (DC \circ \sigma')D_s H' \circ \sigma'. \tag{5.18}$$

This condition must hold for any realizable phase-space path σ'. Certainly this is true if the following condition holds for every phase-space point:

$$D_s H \circ C = DC \cdot (D_s H'). \tag{5.19}$$

Any transformation that satisfies equation (5.19) is a canonical transformation among phase-space representations of a dynamical system. In one phase-space representation the system's dynamics is characterized by the Hamiltonian H' and in the other by H. The idea behind this equation is illustrated in figure 5.1.

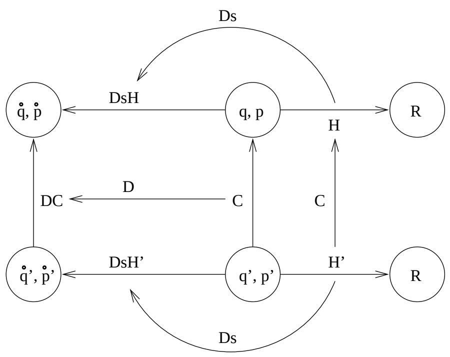

Figure 5.1 A canonical transformation C relates the descriptions of a dynamical system in two phase-space coordinate systems. The transformation shows how Hamilton's equations in one coordinate system may be derived from Hamilton's equations in the other coordinate system.

We can formalize this test as a program:

```
(define (canonical? C H Hprime)
  (- (compose (phase-space-derivative H) C)
     (* (D C) (phase-space-derivative Hprime))))
```

where `phase-space-derivative`, which was introduced in chapter 3, implements D_s. The transformation is canonical if these residuals are zero.

If a suitable Hamiltonian for the transformed system is obtained by composing H with the phase space transformation, we obtain a more specific formula:

$$D_s H \circ C = DC\, D_s(H \circ C). \tag{5.20}$$

and a more specific test

```
(define (compositional-canonical? C H)
  (canonical? C H (compose H C)))
```

Using this test we can verify that the polar-to-rectangular transformation satisfies the test for a canonical transformation on a general central field:

```
(pe
 ((compositional-canonical?
   (F->CT p->r)
   (H-central 'm (literal-function 'V)))
  (->H-state 't
             (coordinate-tuple 'r 'phi)
             (momentum-tuple 'p_r 'p_phi))))
(up 0 (up 0 0) (down 0 0))
```

The residuals are zero so the transformation is canonical.

5.2.1 Time-independent Canonical Transformations

We have defined a canonical transformation as a transformation of phase space coordinates for which Hamilton's equations transform appropriately. The conditions that a canonical transformation must satisfy (equations 5.19 or 5.20) involve the Hamiltonians. If the Hamiltonians transform by composition and the transformation is time-independent then we can tell if the phase space transformation is canonical without further reference to the Hamiltonian.

First, we reformulate Hamilton's equations in a slightly different form. Hamilton's equations are constructed from the derivative of the Hamiltonian by rearranging the components and then negating some of them. We introduce a shuffle function that does this rearrangment:

$$\widetilde{J}([a, b, c]) = (0, c, -b) . \tag{5.21}$$

The argument to $\widetilde{J}$ is a down tuple of components of the derivative of a Hamiltonian-like function. The shuffle function is linear. We also introduce a constant function:

$$\widetilde{T}([a, b, c]) = (1, 0, 0) . \tag{5.22}$$

With these Hamilton's equations can be expressed

$$D\sigma = (\widetilde{J} + \widetilde{T}) \circ DH \circ \sigma. \tag{5.23}$$

Using $\widetilde{J}$ the canonical condition (5.20) can be rewritten

$$\begin{aligned}(\widetilde{J} + \widetilde{T}) \circ (DH) \circ C &= DC \cdot ((\widetilde{J} + \widetilde{T}) \circ (D(H \circ C))) &(5.24)\\ &= DC \cdot (\widetilde{J} \circ ((DH \circ C) \cdot (DC)))\\ &\quad + DC \cdot (\widetilde{T} \circ (D(H \circ C))) &(5.25)\end{aligned}$$

The value of $\widetilde{T}$ does not depend on its arguments, and for time-independent transformations $\widetilde{T} = DC \cdot \widetilde{T}$, so the canonical condition becomes

$$\widetilde{J} \circ (DH) \circ C = DC \cdot (\widetilde{J} \circ ((DH \circ C) \cdot (DC))). \tag{5.26}$$

Applied to a particular phase-space state s this is

$$\widetilde{J}(DH(C(s))) = DC(s) \cdot \widetilde{J}(DH(C(s)) \cdot DC(s)). \tag{5.27}$$

Let Φ be a function that takes a multiplier and produces a linear transformation that multiplies the multiplier by the argument to the linear transformation:

$$\Phi(A)(v) = A \cdot v. \tag{5.28}$$

Similarly, let Φ^* be a function that takes a multiplier and produces a linear transformation that multiplies the argument to the linear transformation by the multipler:

$$\Phi^*(A)(p) = p \cdot A. \tag{5.29}$$

Using Φ and Φ^* we can rewrite condition (5.27) as

$$\begin{aligned}&\widetilde{J}(DH(C(s)))\\ &\quad = (\Phi(DC(s)) \circ \widetilde{J} \circ \Phi^*(DC(s)))(DH(C(s))). &(5.30)\end{aligned}$$

This condition is satisfied if

$$\widetilde{J} = \Phi(DC(s)) \circ \widetilde{J} \circ \Phi^*(DC(s)). \tag{5.31}$$

A time-independent transformation is canonical for Hamiltonians that transform by composition if this condition is satisfied.

Note that the condition (5.31) does not refer to the Hamiltonian. This is a remarkable result. Whether a time-independent phase-space transformation preserves the dynamics of Hamilton's equation can be decided without reference to the details of the dynamical system, provided that the Hamiltonians transform by composition with the transformation.

The test is implemented:

```
(define ((time-independent-canonical? C) s)
  ((- J-func
      (compose (Phi ((D C) s))
               J-func
               (Phi* ((D C) s))))
   (compatible-shape s)))

(define ((Phi A) v) (* A v))

(define ((Phi* A) w) (* w A))
```

This procedure tests whether a composition of functions is the same function as $\widetilde{J}$ by computing their difference when applied to a general typical argument.[4] Here they are applied to a structure with the shape of $DH(s)$, for an arbitrary phase-space state s.[5]

For example, consider the following polar-canonical transformation:

$$(t, x, p_x) = C_\alpha\,(t, \theta, I) \tag{5.32}$$

where

$$x = \sqrt{\frac{2I}{\alpha}} \sin\theta \tag{5.33}$$

$$p_x = \sqrt{2\alpha I} \cos\theta. \tag{5.34}$$

[4]It is in principle impossible to generally determine if two functions are the same, but in this case, since $\Phi(DC(s))$ is linear, this test is valid.

[5]The shape of $DH(s)$ is a *compatible shape* to the shape of s: if they are multiplied the result is a real number. The procedure `compatible-shape` takes any structure and produces another structure that is guaranteed to multiply with the given structure to produce a real number. The structure produced is filled with unique real literals, so if the residual is zero then the functions are the same.

Here α is an arbitrary parameter that we may set to whatever is convenient.

We define:

```
(define ((polar-canonical alpha) H-state)
  (let ((t (state->t H-state))
        (theta (coordinate H-state))
        (I (momentum H-state)))
    (let ((x (* (sqrt (/ (* 2 I) alpha)) (sin theta)))
          (p_x (* (sqrt (* 2 alpha I)) (cos theta))))
      (->H-state t x p_x))))
```

And now we just run our test:

```
(pe
 (time-independent-canonical? (polar-canonical 'alpha)
                              (coordinate-tuple 't 'theta 'I)))
(up 0 0 0)
```

So the transformation is canonical.[6]

Of course, not every transformation we might try is canonical. For example, we might try $x = p \sin \theta$ with $p_x = p \cos \theta$. The implementation is

```
(define (a-non-canonical-transform H-state)
  (let ((t (state->t H-state))
        (theta (coordinate H-state))
        (p (momentum H-state)))
    (let ((x (* p (sin theta)))
          (p_x (* p (cos theta))))
      (->H-state t x p_x))))

(simplify
 (time-independent-canonical? a-non-canonical-transform
                              (->H-state 't 'theta 'p)))

(up 0 (+ (* -1 p x8102) x8102) (+ (* p x8101) (* -1 x8101)))
```

[6] Actually, for $I = 0$ the transform is not well defined and so it is not compositional canonical for that value. This transformation is "locally compositional canonical" in that it is compositional canonical for nonzero values of I. We will ignore this essentially topological problem.

So this transformation is not compositional canonical.[7]

Harmonic Oscillator

The analysis of the harmonic oscillator illustrates the use of a general canonical transformation in the solution of a problem. The harmonic oscillator is the mathematical model of a simple spring-mass system. The Hamiltonian for a spring mass system with mass m and spring constant k is

$$H(t, x, p_x) = \frac{p_x^2}{2m} + \frac{1}{2}kx^2. \tag{5.35}$$

Hamilton's equations of motion are

$$\begin{aligned} Dx &= p_x/m \\ Dp_x &= -kx, \end{aligned} \tag{5.36}$$

giving the second order system

$$mD^2x + kx = 0. \tag{5.37}$$

The solution is

$$x(t) = A\sin(\omega t + \phi), \tag{5.38}$$

where

$$\omega = \sqrt{k/m} \tag{5.39}$$

and where A and ϕ are determined by initial conditions.

Let's try our polar-canonical transformation C_α on the harmonic oscillator. We substitute expressions (5.33) and (5.34) for x and p_x in the Hamiltonian, getting our new Hamiltonian:

$$H'(t, \theta, I) = \frac{\alpha I}{m}(\cos\theta)^2 + \frac{kI}{\alpha}(\sin\theta)^2. \tag{5.40}$$

If we choose $\alpha = \sqrt{km}$ then we obtain

$$H'(t, \theta, I) = \sqrt{\frac{k}{m}}I = \omega I, \tag{5.41}$$

[7] The mysterious symbols such as `x8102` are unique real literals introduced to test functional equalities. That they appeared in a residual demonstrates that the equality is invalid.

and the new Hamiltonian no longer depends on the coordinate. Hamilton's equation for I is

$$DI(t) = -\partial_1 H'(t, \theta(t), I(t)) = 0, \tag{5.42}$$

so I is constant. The equation for θ is

$$D\theta(t) = \partial_2 H'(t, \theta(t), I(t)) = \omega. \tag{5.43}$$

So

$$\theta(t) = \omega t + \phi. \tag{5.44}$$

In the original variables

$$\begin{aligned} x(t) &= \sqrt{2I(t)/\alpha}\sin\theta(t) \\ &= A\sin(\omega t + \phi), \end{aligned} \tag{5.45}$$

with the constant $A = \sqrt{2I(t)/\alpha}$. So we have found the solution to the problem by making a canonical transformation to new phase space variables for which the solution is trivial and then transforming the solutions back to the original variables.

Exercise 5.2: Trouble in Lagrangian World

Is there a Lagrangian L' that corresponds to the harmonic oscillator Hamiltonian $H'(t, \theta, I) = \omega I$? What could this possibly mean?

Exercise 5.3: Polar-Canonical Transformations

Let x, p and θ, I be two sets of canonically conjugate variables. Consider transformations of the form $x = \beta I^\alpha \sin\theta$ and $p = \beta I^\alpha \cos\theta$. Determine all α and β for which this transformation is compositional canonical.

Exercise 5.4: Standard Map

Is the standard map a canonical transformation? Recall the standard map is: $I' = I + K\sin\theta$, with $\theta' = \theta + I'$, both modulo 2π.

5.2.2 Symplectic Transformations

Condition (5.31) involves the composition of functions, all of which are linear transformations. Linear transformations can be represented in terms of matrices. A matrix representation is defined with respect to a basis. For incremental Hamiltonian states we organize the state components as a column matrix of time, the components of the coordinates, and the corresponding components of the momenta.

Let $\widetilde{\mathbf{J}}$ and $\mathbf{DC}$ be the matrix representations of $\widetilde{J}$ and $\Phi(DC(s))$, respectively, and where s is the arbitrary phase-space state at which the canonical condition is being tested. The matrix representation of $\Phi^*(DC(s))$ is the transpose of $\mathbf{DC}$. In terms of these matrix representations the test for canonical becomes

$$\widetilde{\mathbf{J}} = \mathbf{DC}\ \widetilde{\mathbf{J}}\ \mathbf{DC}^{\mathrm{T}}. \tag{5.46}$$

We say that a transformation is *symplectic* if the matrix representation of its derivative satisfies this identity.

The matrix representation of the multiplier for the linear transformation $\widetilde{J}$ is $\widetilde{\mathbf{J}}$. We can find the multipler for a linear transformation by taking the derivative of the linear transformation and evaluating it at an arbitrary point:[8] $D\widetilde{J}([a, b, c])$. We can obtain a matrix representation with the utility `s->m` that takes a multiplier of a linear transformation and returns a matrix representation of the multiplier.[9] The matrix $\widetilde{\mathbf{J}}$ depends only on the number of degrees of freedom. For example, the $\widetilde{\mathbf{J}}$ for a system with two degrees of freedom is:

```
(print-expression
 (let* ((s (typical-H-state 2))
        (s* (compatible-shape s)))
   (s->m s* ((D J-func) s*) s*)))
(matrix-by-rows (list 0 0 0 0 0)
                (list 0 0 0 1 0)
                (list 0 0 0 0 1)
                (list 0 -1 0 0 0)
                (list 0 0 -1 0 0))
```

In terms of matrix representations, the test that a transformation is symplectic is:

---

[8] The derivative of a linear transformation is a constant function, independent of the argument.

[9] The procedure `s->m` takes three arguments: `(s->m` s^* A s`)`. The s^* and s specify the shapes of objects that multiply A on the left and right to give a numerical value; these specify the basis.

```
(define ((symplectic? C) s)
  (let ((s* (compatible-shape s)))
    (let ((J (s->m s* ((D J-func) s*) s*))
          (DCs (s->m s* ((D C) s) s)))
      (- J (* DCs J (m:transpose DCs))))))
```

For example, we can verify that the point transformation derived from the coordinate transformation `p->r` is symplectic:

```
(print-expression
 ((symplectic? (F->CT p->r))
  (->H-state 't
             (coordinate-tuple 'r 'varphi)
             (momentum-tuple 'p_r 'p_varphi))))
(matrix-by-rows (list 0 0 0 0 0)
                (list 0 0 0 0 0)
                (list 0 0 0 0 0)
                (list 0 0 0 0 0)
                (list 0 0 0 0 0))
```

There is a further simplification available. The elements of the first row and the first column of the matrix representation of $\widetilde{J}$ are all zeros. So the first and column of the matrix identity is always satisfied. So we can consider only the submatrix associated with the coordinates and the momenta.

The qp submatrix[10] of dimension $2n \times 2n$ of the matrix $\widetilde{\mathbf{J}}$ is called the symplectic unit for n degrees of freedom:

$$\mathbf{J}_n = \begin{bmatrix} \mathbf{0}_{n\times n} & \mathbf{1}_{n\times n} \\ -\mathbf{1}_{n\times n} & \mathbf{0}_{n\times n} \end{bmatrix}. \tag{5.47}$$

The matrix $\mathbf{J}_n$ satisfies the following identities:

$$\mathbf{J}_n^{\mathrm{T}} = \mathbf{J}_n^{-1} = -\mathbf{J}_n. \tag{5.48}$$

A $2n \times 2n$ matrix $\mathbf{A}$ that satisfies the relation

$$\mathbf{J}_n = \mathbf{A}\mathbf{J}_n\mathbf{A}^{\mathrm{T}} \tag{5.49}$$

[10] The qp submatrix of a $2n + 1$-dimensional square matrix is the $2n$-dimensional matrix obtained by deleting the first row and the first column of the given matrix. This can be computed by:

```
(define (qp-submatrix m)
  (m:submatrix m 1 (m:num-rows m) 1 (m:num-cols m)))
```

is called a *symplectic matrix.*

Here is an alternate test for whether a transformation is symplectic:

```
(define ((symplectic-transform? C) s)
  (symplectic-matrix?
   (qp-submatrix
    (s->m (compatible-shape s)
          ((D C) s)
          s))))

(define (symplectic-matrix? M)
  (let ((2n (m:dimension M)))
    (let ((J (symplectic-unit (quotient 2n 2))))
      (- J (* M J (m:transpose M))))))
```

The procedure `symplectic-transform?` returns a zero matrix if and only if the transformation being tested passes the symplectic matrix test. An appropriate symplectic unit matrix of a given size is produced by the procedure `symplectic-unit`.

The point transformations are symplectic. For example,

```
(print-expression
 ((symplectic-transform? (F->CT p->r))
  (->H-state 't
             (coordinate-tuple 'r 'theta)
             (momentum-tuple 'p_r 'p_theta))))
(matrix-by-rows (list 0 0 0 0)
                (list 0 0 0 0)
                (list 0 0 0 0)
                (list 0 0 0 0))
```

Exercise 5.5: Symplectic matrices

Let $\mathbf{A}$ be a symplectic matrix: $\mathbf{J}_n = \mathbf{A}\mathbf{J}_n\mathbf{A}^{\mathsf{T}}$. Show that $\mathbf{A}^{\mathsf{T}}$ and $\mathbf{A}^{-1}$ are symplectic.

Exercise 5.6: Whittaker Transform

Shew that the transformation $q = \log\left(\frac{1}{q'}\sin p'\right)$ with $p = q'\cot p'$ is symplectic.

5.2.3 Time-Dependent Transformations

We have found that time-independent transformations (involving the coordinates and conjugate momenta, but not the time) are canonical if the derivative of the transformation is symplectic. In this section we re-address the question of when a transformation is canonical, specifically with time dependent transformations in mind. Let's return to the calculation of the symplectic condition, but now allow explicit time dependence in the transformation equations.

If the transformation is time-dependent, then it turns out that $H \circ C$ does not make a suitable H'. Instead, we assume

$$H' = H \circ C + K, \tag{5.50}$$

and look for conditions on K and C that guarantee the transformation is canonical. Equation (5.25), the condition that a transformation is canonical, becomes

$$\begin{aligned}(\widetilde{J} + \widetilde{T}) \circ (DH) \circ C = DC \cdot (\widetilde{J} \circ ((DH \circ C) \cdot DC + DK)) \\ + DC \cdot (\widetilde{T} \circ ((D(H \circ C)) + DK)).\end{aligned} \tag{5.51}$$

This condition is satisfied if the following two conditions are satisfied:

$$\widetilde{J} \circ (DH) \circ C = DC \cdot (\widetilde{J} \circ ((DH \circ C) \cdot (DC))) \tag{5.52}$$

and

$$\begin{aligned}\widetilde{T} \circ (DH) \circ C &= DC \cdot ((\widetilde{J} + \widetilde{T}) \circ (DK)) \\ &= DC \cdot (\widetilde{J} \circ (DK)) + \partial_0 C\end{aligned} \tag{5.53}$$

Condition (5.52) is the condition that C is a symplectic transformation. The second condition is an auxilliary condition on K. This condition does not actually depend on the Hamiltonian H because the constant value of $\widetilde{T}$ does not depend on the argument. The time component is always satisfied; only the coordinate and momentum components of this condition constrain K. Evaluated at a particular state s (with compatible shape s^*) the condition on K is

$$\widetilde{T}(s^*) = DC(s) \cdot (\widetilde{J}(DK(s)) + \partial_0 C(s), \tag{5.54}$$

explicitly showing that the Hamiltonian H does not enter.

Thus we can conclude that a time-dependent transformation is canonical if its position-momentum part is symplectic and if we form the new Hamiltonian by adding an appropriate piece. Note that we have not proven that the position-momentum part must be symplectic. Rather we have shown that if this part is symplectic then the Hamiltonian must be modified in an appropriate way.

As a program, the test for K is

```
(define ((canonical-K? C K) s)
  (let ((s* (compatible-shape s)))
    (- (T-func s*)
       (+ (* ((D C) s) (J-func ((D K) s)))
          (((partial 0) C) s)))))
```

Rotating Coordinates

Consider a time-dependent point transformation to uniformly rotating coordinates:

$$q = R(\Omega)(t, q'), \tag{5.55}$$

with components

$$\begin{aligned} x &= x' \cos(\Omega t) - y' \sin(\Omega t) \\ y &= x' \sin(\Omega t) + y' \cos(\Omega t). \end{aligned} \tag{5.56}$$

As a program this is

```
(define ((rotating Omega) t q)
  (let ((x (ref q 0)) (y (ref q 1)) (z (ref q 2)))
    (coordinate-tuple
      (- (* (cos (* Omega t)) x) (* (sin (* Omega t)) y))
      (+ (* (cos (* Omega t)) y) (* (sin (* Omega t)) x))
      z)))
```

The extension of this transformation to a phase space transformation is

```
(define (C-rotating Omega) (F->CT (rotating Omega)))
```

For this transformation the appropriate correction to the Hamiltonian is

$$K(\Omega)(t; x', y', z'; p'_x, p'_y, p'_z) = -\Omega(x'p'_y - y'p'_x), \tag{5.57}$$

which is the rate of rotation of the coordinate system multiplied by the angular momentum. The justification for this will be given in section 5.3. The implementation is:

```
(define ((K Omega) s)
  (let ((q (coordinate s)) (p (momentum s)))
    (let ((x (ref q 0)) (y (ref q 1))
          (px (ref p 0)) (py (ref p 1)))
      (* -1 Omega (- (* x py) (* y px))))))
```

Applying the test:[11]

```
(pe ((canonical-K? (C-rotating 'Omega) (K 'Omega)) a-state))
(up 0 (up 0 0 0) (down 0 0 0))
```

The residuals are zero so this K completes the canonical transformation.

5.2.4 The Symplectic Condition

A transformation is symplectic if the pq part of the transformation has symplectic derivative. This condition can be written simply in terms of Poisson brackets.

The Poisson bracket can be written in terms of $\widetilde{J}$:

$$\{f, g\} = (Df) \cdot (\widetilde{J} \circ (Dg)), \tag{5.58}$$

as can be seen by writing out the components.

We break the transformation C into position and momentum parts:

$$q = A(t, q', p') \tag{5.59}$$
$$p = B(t, q', p'). \tag{5.60}$$

In terms of the individual component functions the symplectic condition (5.31) is

$$\begin{aligned} \delta^i_j &= \{A^i, B_j\} \\ 0 &= \{A^i, A^j\} \\ 0 &= \{B_i, B_j\} \end{aligned} \tag{5.61}$$

[11] The a-state is:

```
(define a-state
  (->H-state 't
             (coordinate-tuple 'x 'y 'z)
             (momentum-tuple 'p_x 'p_y 'p_z)))
```

where δ^i_j is one if $i = j$ and zero otherwise. These are called the *fundamental Poisson brackets*. If a transformation satisfies these fundamental Poisson bracket relations then it is symplectic.

A time-dependent transformation is canonical if its position-momentum part is symplectic and we modify the Hamiltonian by the addition of a suitable K. We can rewrite these conditions in terms of Poisson brackets. If the Hamiltonian is

$$H'(t, q', p') = H(t, A(t, q', p'), B(t, q', p')) + K(t, q', p'), \tag{5.62}$$

the transformation will be canonical if the coordinate-momentum transformation satisfies the fundamental Poisson brackets, and K satisfies:

$$\begin{aligned} &\{A^i, K\} + \partial_0 A^i = 0 \\ &\{B_j, K\} + \partial_0 B_j = 0. \end{aligned} \tag{5.63}$$

Exercise 5.7:

Fill in the details to show that the symplectic condition (5.31) is equivalent to the fundamental Poisson brackets (5.61) and that the condition on K (5.53) is equivalent to the Poisson bracket condition on K (5.63).

5.3 Generating Functions

We have considered a number of properties of general canonical transformations, without having a general method for coming up with them. Here we introduce the method of *generating functions*. The generating function is a real-valued function which compactly specifies a canonical transformation through its partial derivatives, as follows.

Consider a real-valued function $F_1(t, q, q')$ mapping configurations expressed in two coordinate systems to the reals. We will use F_1 to construct a canonical transformation from one coordinate system to the other. We will show that the following relations among the coordinates, the momenta, and the Hamiltonians specify a canonical transformation:

$$p = \partial_1 F_1(t, q, q') \tag{5.64}$$

$$p' = -\partial_2 F_1(t, q, q') \tag{5.65}$$

$$H'(t, q', p') - H(t, q, p) = \partial_0 F_1(t, q, q'). \tag{5.66}$$

The transformation will then be explicitly given by solving for one set of variables in terms of the others: To obtain the primed variables in terms of the unprimed ones, let A be the inverse of $\partial_1 F_1$ with respect to the third argument,[12]

$$q' = A(t, q, \partial_1 F_1(t, q, q')), \tag{5.67}$$

then

$$q' = A(t, q, p) \tag{5.68}$$
$$p' = -\partial_2 F_1(t, q, A(t, q, p)). \tag{5.69}$$

Let B be the coordinate part of the phase space transformation $q = B(t, q', p')$. This B is an inverse function of $\partial_2 F_2$, satisfying

$$q = B(t, q', -\partial_2 F_1(t, q, q')). \tag{5.70}$$

Using B we have and

$$q = B(t, q', p') \tag{5.71}$$
$$p = \partial_1 F_1(t, B(t, q', p'), q'). \tag{5.72}$$

To put the transformation in explicit form requires that the inverse functions A and B exist.

We can use the above relations to verify that some given transformation from one set of phase space coordinates (q, p) with Hamiltonian function $H(t, q, p)$ to another set (q', p') with Hamiltonian function $H'(t, q', p')$ is canonical by finding an $F_1(t, q, q')$ such that the above relations are satisfied. We can also use arbitrarily chosen generating functions of type F_1 to generate new canonical transformations.

The polar-canonical transformation

The polar-canonical transformation (5.32) from coordinate and momentum (x, p_x) to new coordinate and new momentum (θ, I)

$$x = \sqrt{\frac{2I}{\alpha}} \sin\theta \tag{5.73}$$
$$p_x = \sqrt{2I\alpha} \cos\theta. \tag{5.74}$$

[12] The A and B functions in this section are not the same as those in the previous section.

introduced earlier is canonical. This can also be demonstrated by finding a suitable F_1 generating function. The generating function satisfies a set of partial differential equations (5.64) and (5.65):

$$
\begin{aligned}
p_x &= \partial_1 F_1(t, x, \theta) && (5.75)\\
I &= -\partial_2 F_1(t, x, \theta). && (5.76)
\end{aligned}
$$

Using the relations (5.73) and (5.74), which specify the canonical transformation, the first equation (5.75) can be rewritten

$$p_x = x\alpha \cot\theta = \partial_1 F_1(t, x, \theta), \tag{5.77}$$

which is easily integrated to yield

$$F_1(t, x, \theta) = \frac{\alpha}{2} x^2 \cot\theta + \phi(t, \theta) \tag{5.78}$$

where ϕ is some integration "constant" with respect to the first integration. Substituting this form for F_1 into the second partial differential equation (5.76) we find

$$I = -\partial_2 F_1(t, x, \theta) = \frac{\alpha}{2} \frac{x^2}{\sin^2\theta} - \partial_1 \phi(t, \theta) \tag{5.79}$$

but we see that if we set $\phi = 0$, the desired relations are recovered. So the generating function

$$F_1(t, x, \theta) = \frac{\alpha}{2} x^2 \cot\theta \tag{5.80}$$

generates the polar-canonical transformation. This shows that this transformation is canonical.

5.3.1 F_1 Generates Canonical Transformations

We can prove directly that the transformation generated by F_1 is canonical by showing that if Hamilton's equations are satisfied in one set of coordinates then Hamilton's equations will be satisfied in the other set of coordinates. Let F_1 take arguments (t, x, y). The relations among the coordinates are

$$
\begin{aligned}
p_x &= \partial_1 F_1(t, x, y)\\
p_y &= -\partial_2 F_1(t, x, y) && (5.81)
\end{aligned}
$$

and the Hamiltonians are related by

$$H'(t, y, p_y) = H(t, x, p_x) + \partial_0 F_1(t, x, y). \tag{5.82}$$

Substituting the generating function relations (5.81) into this equation, we have

$$H'(t, y, -\partial_2 F_1(t, x, y)) = H(t, x, \partial_1 F_1(t, x, y)) + \partial_0 F_1(t, x, y). \tag{5.83}$$

Take the partial derivatives of this equality of expressions with respect to the variables x and y:[13]

$$\begin{aligned} -(\partial_2 H')^j (\partial_1(\partial_2 F_1)_j)_i &= (\partial_1 H)_i + (\partial_2 H)^j (\partial_1(\partial_1 F_1)_j)_i + (\partial_1 \partial_0 F_1)_i \\ (\partial_1 H')_i - (\partial_2 H')^j (\partial_2(\partial_2 F_1)_j)_i &= (\partial_2 H)^j (\partial_2(\partial_1 F_1)_j)_i + (\partial_2 \partial_0 F_1)_i \end{aligned} \tag{5.84}$$

where the arguments are unambiguous and have been suppressed. On solution paths we can use Hamilton's equations for the (x, p_x) system to replace the partial derivatives of H with derivatives of x and p_x, obtaining

$$\begin{aligned} -(\partial_2 H')^j (\partial_1(\partial_2 F_1)_j)_i &= -(Dp_x)_i + (Dx)^j (\partial_1(\partial_1 F_1)_j)_i + (\partial_1 \partial_0 F_1)_i \\ (\partial_1 H')_i - (\partial_2 H')^j (\partial_2(\partial_2 F_1)_j)_i &= (Dx)^j (\partial_2(\partial_1 F_1)_j)_i + (\partial_2 \partial_0 F_1)_i. \end{aligned} \tag{5.85}$$

Now compute the derivative of p_x and p_y, from equations (5.81), along consistent paths

$$\begin{aligned} (Dp_x)_i &= (\partial_1(\partial_1 F_1)_i)_j (Dx)^j + (\partial_2(\partial_1 F_1)_i)_j (Dy)^j + \partial_0(\partial_1 F_1)_i \\ (Dp_y)_i &= -(\partial_1(\partial_2 F_1)_i)_j (Dx)^j - (\partial_2(\partial_2 F_1)_i)_j (Dy)^j - \partial_0(\partial_2 F_1)_i. \end{aligned} \tag{5.86}$$

Substituting the first of these into the first of equations (5.85)

$$-(\partial_2 H')^j (\partial_1(\partial_2 F_1)_j)_i = -(\partial_1(\partial_2 F_1)_j)_i (Dy)^j. \tag{5.87}$$

[13] Here we use indices to select particular components of structured objects. If an index symbol appears both as a superscript and as a subscript in an expression, the value of the expression is the sum over all possible values of the index symbol of the designated components (Einstein summation convention). Thus, for example, if $\dot{q}$ and p are of dimension n then the indicated product $p_i \dot{q}^i$ is to be interpreted as $\Sigma_{i=0}^{n-1} p_i \dot{q}^i$.

Note that $(\partial_2(\partial_1 F_1)_i)_j = (\partial_1(\partial_2 F_1)_j)_i$. Provided that $\partial_2\partial_1 F_1$ is non-singular,[14] we have derived one of Hamilton's equations for the (y, p_y) system

$$Dy(t) = \partial_2 H'(t, y(t), p_y(t)). \tag{5.88}$$

The other Hamilton's equation,

$$Dp_y(t) = -\partial_1 H'(t, y(t), p_y(t)), \tag{5.89}$$

can be derived in a similar way. So the generating function relations indeed specify a canonical transformation.

What we have shown is that the transformation is canonical, which means that the equations of motion transform appropriately; we have not shown that the qp part of the transformation is symplectic. If the transformation is time-independent then the Hamiltonians transform by composition, and in that circumstance we know that canonical implies symplectic.

5.3.2 Other Generating Functions

We have used F_1 type generating functions to construct canonical transformations:

$$p = \partial_1 F_1(t, q, q') \tag{5.90}$$
$$p' = -\partial_2 F_1(t, q, q') \tag{5.91}$$
$$H'(t, q', p') - H(t, q, p) = \partial_0 F_1(t, q, q'). \tag{5.92}$$

We can also represent canonical transformations with generating functions of the form $F_2(t, q, p')$, where the third argument of F_2 is the momentum in the primed system.[15] The generating functions F_1 and F_2 are related by a Legendre transform as follows:

$$p' = -\partial_2 F_1(t, q, q') \tag{5.93}$$
$$p'q' = -F_1(t, q, q') + F_2(t, q, p') \tag{5.94}$$

[14] A structure is non-singular if the determinant of the matrix representation of the structure is non-zero.

[15] The various generating functions are traditionally known by the names: F_1, F_2, F_3, and F_4. Please don't blame us.

$$q' = \partial_2 F_2(t, q, p'). \tag{5.95}$$

We have passive variables q and t:

$$-\partial_1 F_1(t, q, q') + \partial_1 F_2(t, q, p') = 0 \tag{5.96}$$
$$-\partial_0 F_1(t, q, q') + \partial_0 F_2(t, q, p') = 0 \tag{5.97}$$

But $p = \partial_1 F_1(t, q, q')$ from the first transformation, so

$$p = \partial_1 F_2(t, q, p'). \tag{5.98}$$

Furthermore, since $H'(t, q', p') - H(t, q, p) = \partial_0 F_1(t, q, q')$ we can conclude that:

$$H'(t, q', p') - H(t, q, p) = \partial_0 F_2(t, q, p') \tag{5.99}$$

In summary, the following equations specify a canonical transformation:

$$p = \partial_1 F_2(t, q, p') \tag{5.100}$$
$$q' = \partial_2 F_2(t, q, p') \tag{5.101}$$
$$H'(t, q', p') - H(t, q, p) = \partial_0 F_2(t, q, p') \tag{5.102}$$

As in the F_1 case to put the transformation in explicit form requires that appropriate inverse functions be constructed to allow the solution of the equations.

Similarly, we can construct two other forms for generating functions, named mnemonically enough F_3 and F_4:

$$q = -\partial_1 F_3(t, p, q') \tag{5.103}$$
$$p' = -\partial_2 F_3(t, p, q') \tag{5.104}$$
$$H'(t, q', p') - H(t, q, p) = \partial_0 F_3(t, p, q') \tag{5.105}$$

and

$$q = -\partial_1 F_4(t, p, p') \tag{5.106}$$
$$q' = \partial_2 F_4(t, p, p') \tag{5.107}$$
$$H'(t, q', p') - H(t, q, p) = \partial_0 F_4(t, p, p') \tag{5.108}$$

In every case, if the generating function does not depend explicitly on time then the Hamiltonians are obtained from each other purely by composition with the appropriate canonical transformation. If the generating function depends on time, then there are additional terms.

The generating functions presented treat the coordinates and momenta collectively. One could define more complicated generating functions for which the transformation of each degree of freedom is specified by generating functions of different types.

5.3.3 Point transformations

Point transformations can be represented in terms of a generating function of type F_2. The equations (5.6) which define a canonical point transformation derived from a coordinate transformation F are:

$$(t, q, p) = C\,(t, q', p') = \left(t, F(t, q'), p'(\partial_1 F(t, q'))^{-1}\right) \tag{5.109}$$

Let S be the inverse transformation of F with respect to the second argument

$$q' = S(t, q), \tag{5.110}$$

so that $q' = S(t, F(t, q'))$. The momentum transformation that accompanies this coordinate transformation is

$$p' = p(\partial_1 S(t, q))^{-1}. \tag{5.111}$$

We can find the generating function F_2 that gives this transformation by integrating equation (5.101):

$$q' = \partial_2 F_2(t, q, p'), \tag{5.112}$$

to get

$$F_2(t, q, p') = p' S(t, q) + \phi(t, q). \tag{5.113}$$

Substituting this into equation (5.100):

$$p = \partial_1 F_2(t, q, p'), \tag{5.114}$$

we get

$$p = p' \partial_1 S(t, q) + \partial_1 \phi(t, q). \tag{5.115}$$

We do not need the freedom provided by ϕ so we can set it equal to zero:

$$F_2(t, q, p') = p' S(t, q), \tag{5.116}$$

with

$$p = p' \partial_1 S(t, q). \tag{5.117}$$

So this F_2 gives the canonical transformation of equations (5.110) and (5.111).

The canonical transformation for the coordinate transformation S is the inverse of the canonical transformation for F. By design F and S are inverses on the coordinate arguments. The identity function is $q' = I(q') = S(t, F(t, q'))$. Differentiating yields

$$1 = \partial_1 S(t, F(t, q')) \partial_1 F(t, q'), \tag{5.118}$$

so

$$\partial_1 F(t, q') = (\partial_1 S(t, F(t, q')))^{-1}. \tag{5.119}$$

Using this, the relation between the momenta (5.117) is

$$p = p' (\partial_1 F(t, q'))^{-1}, \tag{5.120}$$

showing that F_2 gives a point transformation equivalent to the point transformation (5.109)

So from this other point of view we see that the point transformation is canonical.

The F_1 that corresponds to the F_2 for a point transformation is:

$$\begin{aligned} F_1(t, q, q') &= F_2(t, q, p') - p'q' \\ &= p' S(t, q) - p'q' \\ &= 0. \end{aligned} \tag{5.121}$$

This shows that there is no one-to-one relationship between generating functions of a particular type and canonical transformations: all point transformations have the same F_1.[16]

Polar and Rectangular Coordinates

A commonly required point transformation is the transition between polar coordinates and rectangular coordinates:

$$\begin{aligned} x &= r\cos\theta \\ y &= r\sin\theta. \end{aligned} \tag{5.122}$$

Using the formula for the generating function of a point transformation just derived:

$$F_2(t;r,\theta;p_x,p_y) = [\,p_x \quad p_y\,]\begin{pmatrix} r\cos\theta \\ r\sin\theta \end{pmatrix}. \tag{5.123}$$

So the full transformation is derived:

$$\begin{aligned} (x,y) &= \partial_2 F_2(t;r,\theta;p_x,p_y) \\ &= (r\cos\theta, r\sin\theta) \\ [p_r,p_\theta] &= \partial_1 F_2(t;r,\theta;p_x,p_y) \\ &= [p_x\cos\theta + p_y\sin\theta, -p_x r\sin\theta + p_y r\cos\theta]\,. \end{aligned} \tag{5.124}$$

We can isolate the rectangular coordinates to one side of the transformation and the polar coordinates to the other

$$\begin{aligned} p_r &= \frac{1}{r}(p_x x + p_y y) \\ p_\theta &= -p_x y + p_y x. \end{aligned} \tag{5.125}$$

So, interpreted in terms of Newtonian vectors, $p_r = \hat{r}\cdot\vec{p}$ is the radial component of the linear momentum and $p_\theta = ||\vec{r}\times\vec{p}||$ is the magnitude of the angular momentum. Since the point transfor-

---

[16] This also shows that the reasoning that led to the conclusion that the F_2 generating function relations specify a canonical transformation, using the Legendre transform relations, was inadequate. That argument started from the F_1 generating function relations, but if F_1 is identically zero those relations do not specify a phase-space transformation. So the argument is wrong. Instead, we should separately show that the F_2 relations specify a canonical transformation, and then show that the F_1 and F_2 relations are related by a Legendre transform, if the transformation relations are non-degenerate.

mation is time independent the Hamiltonian transforms by composition.

Rotating Coordinates

A useful time-dependent point transformation is the transition to a rotating coordinate system. This is most easily accomplished in polar coordinates. Here we have

$$\begin{aligned} r' &= r \\ \theta' &= \theta - \Omega t, \end{aligned} \tag{5.126}$$

where Ω is the angular velocity of the moving frame of reference. The generating function is

$$F_2(t; r, \theta; p'_r, p'_\theta) = [\, p'_r \quad p'_\theta \,] \begin{pmatrix} r \\ \theta - \Omega t \end{pmatrix}. \tag{5.127}$$

This yields the transformation equations

$$\begin{aligned} r' &= r \\ \theta' &= \theta - \Omega t \\ p_r &= p'_r \\ p_\theta &= p'_\theta, \end{aligned} \tag{5.128}$$

which show that the momenta are the same in both coordinate systems. However, here the Hamiltonian is not a simple composition:

$$H'(t; r', \theta'; p'_r, p'_\theta) = H(t; r', \theta' + \Omega t; p'_r, p'_\theta) - p'_\theta \Omega. \tag{5.129}$$

The Hamiltonians differ by the derivative of the generating function with respect to the time argument. In transforming to a rotating frame the values of the Hamiltonians differ by the product of the angular momentum and the angular velocity of the frame. Notice that this addition to the Hamiltonian is the same as was found earlier (5.57).

Two Body Problem

In this example we illustrate how canonical transformations can be used to eliminate some of the degrees of freedom, leaving an essential problem with fewer degrees of freedom. The basic procedure is quite important and will be used over and over.

Suppose only certain combinations of the coordinates appear in the Hamiltonian. We make a canonical transformation to a new set of phase-space coordinates. We choose some of the new coordinates to be those combinations of the original phase-space coordinates that occur in the Hamiltonian. We choose other coordinates to complete the set. These other coordinates do not actually appear in the new Hamiltonian, so the momenta conjugate to them are conserved quantities.

Let's see how this idea lets us reduce the problem of two gravitating bodies to the simpler problem of the relative motion of the two bodies, and in the process discover that the momentum of the center of mass is conserved.

Consider the motion of two masses m_1 and m_2, subject only to a mutual gravitational attraction described by the potential $V(r)$. This problem has six degrees of freedom. The rectangular coordinates of the particles are x_1 and x_2, with conjugate momenta p_1 and p_2. Each of these is a structure of the three rectangular components. The distance between the particles is $r = \|x_1 - x_2\|$. The Hamiltonian for the two-body problem is:

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(r). \tag{5.130}$$

We do not need to further specify V at this point.

We note that the only linear combination of coordinates that appears in the Hamiltonian is $x_2 - x_1$. We choose new coordinates so that one of the new coordinates is this combination

$$x = x_2 - x_1 \tag{5.131}$$

and to complete the set of new coordinates we choose some independent linear combination

$$X = ax_1 + bx_2 \tag{5.132}$$

where a and b are to be determined. We can use an F_2 type generating function

$$F_2(t; x_1, x_2; p, P) = (x_2 - x_1)p + (ax_1 + bx_2)P, \tag{5.133}$$

where p and P will be the new momenta conjugate to x and X, respectively. We deduce

$$\begin{aligned}(x, X) &= \partial_2 F_2(t; x_1, x_2; p, P) = (x_2 - x_1, ax_1 + bx_2)\\ [p_1, p_2] &= \partial_1 F_2(t; x_1, x_2; p, P) = [-p + aP, p + bP]\,.\end{aligned} \tag{5.134}$$

We can solve these for the new momenta:

$$P = \frac{p_1 + p_2}{a + b} \tag{5.135}$$

$$p = \frac{ap_2 - bp_1}{a + b}. \tag{5.136}$$

The generating function is not time dependent so the new Hamiltonian is the old Hamiltonian composed with the transformation:

$$\begin{aligned}H'(t; x, X; p, P) &= \frac{(-p + aP)^2}{2m_1} + \frac{(p + bP)^2}{2m_2} + V(||x||)\\ &= \frac{p^2}{2\mu} + \frac{P^2}{2M} + V(||x||)\\ &\quad + \left(\frac{b}{m_2} - \frac{a}{m_1}\right) pP,\end{aligned} \tag{5.137}$$

with the definitions

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2} \tag{5.138}$$

and

$$\frac{1}{M} = \frac{a^2}{m_1} + \frac{b^2}{m_2}. \tag{5.139}$$

We recognize μ as the usual "reduced mass."

Notice that if the term proportional to pP were not present then the x and X degrees of freedom would not be coupled at all, and furthermore, the X part of the Hamiltonian would be just the Hamiltonian of a free particle which is trivial to solve. The condition that the "cross terms" disappear is

$$\frac{b}{m_2} - \frac{a}{m_1} = 0, \tag{5.140}$$

which is satisfied by

$$a = cm_1 \tag{5.141}$$

$$b = cm_2 \tag{5.142}$$

for any c.[17] So with this choice the Hamiltonian becomes

$$H' = H_X + H_x \tag{5.143}$$

with

$$H_x = \frac{p^2}{2\mu} + V(r) \tag{5.144}$$

and

$$H_X = \frac{P^2}{2M}. \tag{5.145}$$

The reduced mass is the same as before, and now

$$M = \frac{1}{c^2(m_1 + m_2)} \tag{5.146}$$

Notice that without further specifying c the problem has been separated into the problem of determining the relative motion of the two masses, and the problem of the other degrees of freedom. We did not need to have a priori knowledge that the center of mass might be important; and, in fact, only for particular choice of $c = (m_1 + m_2)^{-1}$ does X become the center of mass.[18]

Epicyclic motion

It is often useful to compose a sequence of canonical transformations to make up the transformation we need for any particular mechanical problem. The transformations we have supplied are especially useful as components in these computations.

We will illustrate the use of canonical transformations to learn about planar motion in a central field. The strategy will be to

---

[17] For a transformation to be defined c must be non-zero.

[18] The example was chosen to illustrate this approach for reducing problems to simpler problems. This particular application is not very difficult. The same procedure can be used to do more complicated tasks. For example, the elimination of the overall translational degree of freedom in the n-body can be approached in a similar manner to discover the Jacobi coordinates.

consider perturbations of circular motion in the central field. The analysis will proceed by transforming to a rotating coordinate system that rides on a circular reference orbit, and then to make approximations that restrict the analysis to orbits that differ from the circular orbit only slightly.

Recall that in rectangular coordinates we could easily write a Hamiltonian for the motion of a particle of mass m in a field defined by a potential energy that is only a function of the distance from the origin as follows:

$$H(t; x, y; p_x, p_y) = \frac{p_x^2 + p_y^2}{2m} + V(\sqrt{x^2 + y^2}) \tag{5.147}$$

In this coordinate system Hamilton's equations are easy, and they are exactly what is needed to develop trajectories by numerical integration, but the expressions are not very illuminating:

$$Dx = \frac{p_x}{m} \tag{5.148}$$

$$Dy = \frac{p_y}{m} \tag{5.149}$$

$$Dp_x = -DV(\sqrt{x^2 + y^2})\frac{x}{\sqrt{x^2 + y^2}} \tag{5.150}$$

$$Dp_y = -DV(\sqrt{x^2 + y^2})\frac{y}{\sqrt{x^2 + y^2}} \tag{5.151}$$

We can learn more by converting to polar coordinates centered on the source of our field.

$$x = r \cos \phi \tag{5.152}$$

$$y = r \sin \phi \tag{5.153}$$

This coordinate system explicitly incorporates the geometrical symmetry of the potential energy. Using the results of the previous section we can write the new Hamiltonian as:

$$H'(t; r, \phi; p_r, p_\phi) = \frac{p_r^2}{2m} + \frac{p_\phi^2}{2mr^2} + V(r) \tag{5.154}$$

We can now write Hamilton's equations in these new coordinates, and they are much more illuminating than the equations expressed in rectangular coordinates:

$$Dr = \frac{p_r}{m} \tag{5.155}$$

$$D\phi = \frac{p_\phi}{mr^2} \tag{5.156}$$

$$Dp_r = \frac{p_\phi^2}{mr^3} - DV(r) \tag{5.157}$$

$$Dp_\phi = 0 \tag{5.158}$$

We see that the angular momentum p_ϕ is conserved, and we are free to choose its constant value, so $D\phi$ depends only on r. We also see that we can establish a circular orbit at any radius R_0: we choose $p_\phi = p_{\phi_0}$ so that $\frac{p_{\phi 0}^2}{mR_0^3} - DV(R_0) = 0$. This will ensure that $Dp_r = 0$, and thus $Dr = 0$. The (square of the) angular velocity of this circular orbit is

$$\Omega^2 = \frac{DV(R_0)}{mR_0}. \tag{5.159}$$

It is instructive to consider how orbits that are close to the circular orbit differ from the circular orbit. This is best done in a frame where a body moving in the circular orbit is a stationary point at the origin. We can do this by converting to coordinates that are rotating with the circular orbit and centered on the orbiting body. We will do this in three stages. First we will transform to a polar coordinate system that is rotating at angular velocity Ω. Then we will return to rectangular coordinates, and finally, we will shift the coordinates so the origin is on the reference circular orbit.

We start by examining the system in rotating polar coordinates. This is a time-varying coordinate transformation:

$$r' = r \tag{5.160}$$

$$\phi' = \phi - \Omega t \tag{5.161}$$

$$p'_r = p_r \tag{5.162}$$

$$p'_\phi = p_\phi \tag{5.163}$$

Using the formulas developed in the last section we can now write the new Hamiltonian directly:

$$H''(t; r', \phi'; p'_r, p'_\phi) = \frac{p_r'^2}{2m} + \frac{p_\phi'^2}{2mr'^2} + V(r') - p'_\phi \Omega \tag{5.164}$$

We see that H'' is not time dependent, and therefore it is conserved, but it is not energy. Energy is not conserved in the moving coordinate system, but what is conserved here is a new quantity which combines the energy with the product of the angular momentum of the particle in the new frame and the angular velocity of the frame. We will want to keep track of this term.

Next, we return to rectangular coordinates, but they are rotating with the reference circular orbit:

$$x' = r' \cos \phi' \tag{5.165}$$
$$y' = r' \sin \phi' \tag{5.166}$$
$$p'_x = p'_r \cos \phi' - \frac{p'_\phi}{r'} \sin \phi' \tag{5.167}$$
$$p'_y = p'_r \sin \phi' + \frac{p'_\phi}{r'} \cos \phi'. \tag{5.168}$$

The Hamiltonian is

$$\begin{aligned} &H'''(t; x', y'; p'_x, p'_y) \\ &\quad = \frac{p'^2_x + p'^2_y}{2m} + \Omega(y' p'_x - x' p'_y) + V(\sqrt{x'^2 + y'^2}). \end{aligned} \tag{5.169}$$

With one more quick manipulation we shift the coordinate system so that the origin is out on our circular orbit. We define new rectangular coordinates ξ and η with the following simple canonical transformation of coordinates and momenta:

$$\xi = x' - R_0 \tag{5.170}$$
$$\eta = y' \tag{5.171}$$
$$p_\xi = p'_x \tag{5.172}$$
$$p_\eta = p'_y. \tag{5.173}$$

In this final coordinate system the Hamiltonian is

$$\begin{aligned} H''''(t; \xi, \eta; p_\xi, p_\eta) = &\frac{p^2_\xi + p^2_\eta}{2m} + \Omega(\eta p_\xi - (\xi + R_0) p_\eta) \\ &+ V(\sqrt{(\xi + R_0)^2 + \eta^2}), \end{aligned} \tag{5.174}$$

and Hamilton's equations are uselessly complicated, but the next step is to consider only trajectories for which the coordinates ξ and η are small compared with R_0. Under this assumption we will be able to construct approximate equations of motion for these trajectories that are linear in the coordinates, thus yielding simple analyzable motion. Note that up until here, we have made no approximations. The equations above are perfectly accurate for any trajectories in a central field.

The idea is to expand the potential-energy term in the Hamiltonian as a series and to discard any term higher than second order in the coordinates, thus giving us first-order accurate Hamilton's equations:

$$\begin{aligned} U(\xi,\eta) &= V(\sqrt{(\xi+R_0)^2+\eta^2}) && (5.175)\\ &= V(R_0+\xi+\frac{\eta^2}{2R_0}+\cdots) && (5.176)\\ &= V(R_0)+DV(R_0)(\xi+\frac{\eta^2}{2R_0})\\ &\quad + D^2V(R_0)\frac{\xi^2}{2}+\cdots. && (5.177)\end{aligned}$$

So the (negated) generalized forces are:

$$\begin{aligned} \partial_0 U(\xi,\eta) &= DV(R_0)+D^2V(R_0)\xi+\cdots && (5.178)\\ \partial_1 U(\xi,\eta) &= DV(R_0)\frac{\eta}{R_0}+\cdots. && (5.179)\end{aligned}$$

With this expansion we obtain the linearized Hamilton's equations:

$$\begin{aligned} D\xi &= \frac{p_\xi}{m}+\Omega\eta && (5.180)\\ D\eta &= \frac{p_\eta}{m}-\Omega(\xi+R_0) && (5.181)\\ Dp_\xi &= -DV(R_0)-D^2V(R_0)\xi+\cdots+\Omega p_\eta && (5.182)\\ Dp_\eta &= -DV(R_0)\frac{\eta}{R_0}+\cdots-\Omega p_\xi. && (5.183)\end{aligned}$$

Of course, once we have linear equations we know how to solve them exactly. Since the linearized Hamiltonian is conserved we cannot get exponential expansion or collapse. So the possible solutions are quite limited. It is instructive to convert these equations into a second-order system. We use $\Omega^2 = \frac{DV(R_0)}{mR_0}$ to eliminate the

DV terms:

$$D^2\xi - 2\Omega D\eta = (\Omega^2 - \frac{D^2V(R_0)}{m})\xi \tag{5.184}$$

$$D^2\eta + 2\Omega D\xi = 0. \tag{5.185}$$

Combining these we find

$$D^3\xi + \omega^2 D\xi = 0 \tag{5.186}$$

where

$$\omega^2 = 3\Omega^2 + \frac{D^2V(R_0)}{m}. \tag{5.187}$$

Thus we have a simple harmonic oscillator with frequency ω as one of the components of the solution. The general solution has three parts

$$\begin{bmatrix} \xi(t) \\ \eta(t) \end{bmatrix} = \eta_0 \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{5.188}$$

$$+ \xi_0 \begin{bmatrix} 1 \\ -2At \end{bmatrix} \tag{5.189}$$

$$+ C_0 \begin{bmatrix} \sin(\omega t + \varphi_0) \\ \frac{2\Omega}{\omega}\cos(\omega t + \varphi_0) \end{bmatrix} \tag{5.190}$$

where

$$A = \frac{\Omega^2 m - D^2V(R_0)}{4\Omega m}. \tag{5.191}$$

The constants η_0, ξ_0, C_0, and φ_0 are determined by the initial conditions. If $C_0 = 0$ the particle of interest is on a circular trajectory, but not necessarily the same one as the reference trajectory. If $C_0 = 0$ and $\xi_0 = 0$ we have a "fellow traveler", a particle in the same circular orbit as the reference orbit, but with different phase. If $C_0 = 0$ and $\eta_0 = 0$ we have a particle in a circular orbit that is interior or exterior to the reference orbit and shearing away from the reference orbit. The shearing is due to the fact that the angular velocity for a circular orbit varies with the radius. The constant A gives the rate of shearing at each radius. If both $\eta_0 = 0$ and $\xi_0 = 0$ but $C_0 \neq 0$ then we have "epicyclic motion". A particle in a nearly circular orbit may be seen to move in an ellipse around the circular reference orbit. The ellipse will be elongated in the direction of circular motion by the factor $\frac{2\Omega}{\omega}$ and it will rotate in the direction opposite the direction of the circular motion. The initial phase of the epicycle is φ_0. Of course, any combination of these solutions may exist.

The epicyclic frequency ω and the shearing rate A are determined by the force law (the radial derivative of the potential energy). For a force law proportional to a power of the radius

$$F \propto r^{1-n} \tag{5.192}$$

the epicyclic frequency is related to the orbital frequency by

$$\frac{\omega}{\Omega} = 2\sqrt{1 - \frac{n}{4}} \tag{5.193}$$

and the shearing rate is

$$\frac{A}{\Omega} = \frac{n}{4}. \tag{5.194}$$

For a few particular integer force laws we see:

n	0	1	2	3	4	5
$\frac{A}{\Omega}$	0	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{3}{4}$	1	$\frac{5}{4}$
$\frac{\omega}{\Omega}$	2	$\sqrt{3}$	$\sqrt{2}$	1	0	$\pm i$

We can get some insight into the kinds of orbits that are produced by the epicyclic approximation by examining a few examples. For some force laws we have integer ratios of epicyclic frequency to orbital frequency. In those cases we have closed orbits. For an inverse-square force law ($n = 3$) we get elliptical orbits with the center of the field at a focus of the ellipse. Figure 5.2 shows how an approximation to such an orbit can be constructed by superposition of the motion on an elliptical epicycle with the motion of the same frequency on a circle. If the force is proportional to the radius ($n = 0$) we get a two-dimensional harmonic oscillator. Here the epicyclic frequency is twice the orbital frequency. Figure 5.3 shows how this yields elliptical orbits that are centered on the source of the central force. An orbit is closed when $\frac{\omega}{\Omega}$ is a rational fraction. If the force is proportional to the $-3/4$ power of the radius the epicyclic frequency is $3/2$ the orbital frequency. This yields a 3-lobed pattern that can be seen in figure 5.4. For other force laws the orbits predicted by this analysis are multi-lobed patterns produced by precessing approximate ellipses. Most of the cases have incommensurate epicyclic and orbital frequencies, leading to orbits that do not close in finite time.

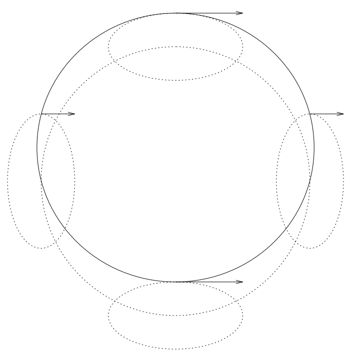

Figure 5.2 Epicyclic construction of an approximate orbit for $F \propto r^{-2}$. The large dotted circle is the reference circular orbit. The dotted ellipses are the epicycles. The epicycles are twice as long as they are wide. The solid ellipse is the approximate trajectory produced by a particle moving on the epicycles. The sense of orbital motion is counterclockwise, and the epicycles are rotating clockwise. The arrows represent the increment of velocity contributed by the epicycle to the circular reference orbit.

The epicyclic approximation gives a very good idea of what actual orbits look like. Figure 5.5, drawn by numerical integration of the orbit produced by integrating the original rectangular equations of motion for a particle in the field, shows the rosette-type picture characteristic of incommensurate epicyclic and orbital frequencies for an $F = -r^{-2.3}$ force law.

We can directly compare a numerically integrated system with one of our epicyclic approximations. For example the result of numerically integrating our $F \propto r^{-3/4}$ system is very similar to the picture we obtained by epicycles. (See figure 5.6 and compare it with figure 5.4.)

Exercise 5.8: Collapsing orbits

What exactly happens as the force law becomes more steep? Investigate this by sketching the contours of the Hamiltonian in r, p_r space, for various values of the force-law exponent, n. For what values of n are

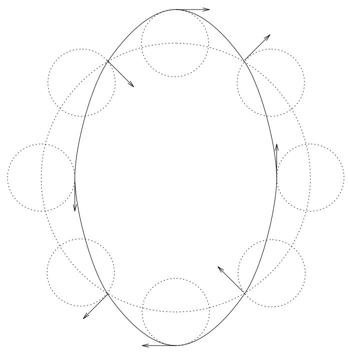

Figure 5.3 Epicyclic construction of an approximate orbit for $F \propto r$. The large dotted circle is the reference circular orbit. The small dotted circles are the epicycles. The solid ellipse is the approximate trajectory produced by a particle moving on the epicycles. The sense of orbital motion is counterclockwise, and the epicycles are rotating clockwise. The arrows represent the increment of velocity contributed by the epicycle to the circular reference orbit.

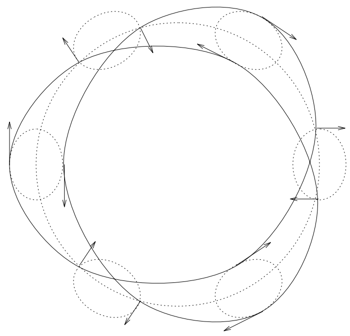

Figure 5.4 Epicyclic construction of an approximate orbit for $F \propto r^{-3/4}$. The large dotted circle is the reference circular orbit. The dotted ellipses are the epicycles. The epicycles are in a 4 : 3 ratio of length to width. The solid ellipse is the approximate trajectory produced by a particle moving on the epicycles. The sense of orbital motion is counterclockwise, and the epicycles are rotating clockwise. The arrows represent the increment of velocity contributed by the epicycle to the circular reference orbit.

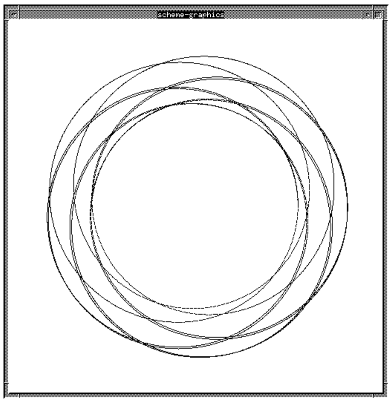

Figure 5.5 The numerically integrated orbit of a particle with a force law $F \propto r^{-2.3}$. For this law the ratio of the epicyclic frequency to the orbital frequency is about .83666—close to 5/6, but not quite. This is manifest in the nearly 5-fold symmetry of the rosette-like shape and the fact that one must cross approximately six orbits to get from the inside to the outside of the rosette.

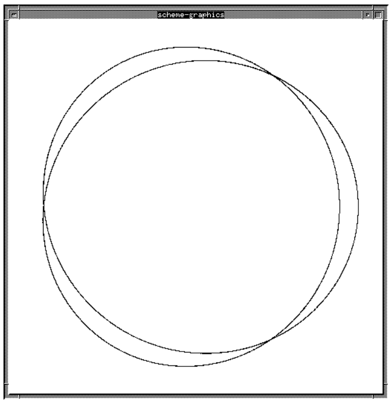

Figure 5.6 The numerically integrated orbit of a particle with a force law $F \propto r^{-3/4}$. For this law the ratio of the epicyclic frequency to the orbital frequency is exactly 3/2. This is manifest in the 3-fold symmetry of the rosette-like shape and the fact that one must cross two orbits to get from the inside to the outside of the rosette.

there stable circular orbits? In the case that there are no stable circular orbits what happens to circular and other noncircular orbits? How are these results consistent with Liouville's theorem and the non-existence of attractors in Hamiltonian systems.

5.3.4 Classical "Gauge" Transformations

The addition of a total time derivative to a Lagrangian leads to the same Lagrange equations. However, the two Lagrangians have different momenta, and they lead to different Hamilton's equations. Here, we find out how to represent the corresponding canonical transformation with a generating function.

Let's restate the result about total time derivatives and Lagrangians from the first chapter. Consider some function $G(t, q)$ of time and coordinates. We have shown that if L and L' are related by

$$L'(t, q, \dot{q}) = L(t, q, \dot{q}) + \partial_0 G(t, q) + \partial_1 G(t, q)\dot{q} \tag{5.195}$$

then the Lagrange equations of motion are the same. The generalized coordinates used in the two Lagrangians are the same, but the momenta conjugate to the coordinates are different. In the usual way, define

$$\mathcal{P}(t, q, \dot{q}) = \partial_2 L(t, q, \dot{q}) \tag{5.196}$$

and

$$\mathcal{P}'(t, q, \dot{q}) = \partial_2 L'(t, q, \dot{q}). \tag{5.197}$$

So we have

$$\mathcal{P}'(t, q, \dot{q}) = \mathcal{P}(t, q, \dot{q}) + \partial_1 G(t, q). \tag{5.198}$$

Evaluated on a trajectory, we have

$$p'(t) = p(t) + \partial_1 G(t, q(t)). \tag{5.199}$$

This transformation is a special case of an F_2 type transformation. Let

$$F_2(t, q, p') = qp' - G(t, q), \tag{5.200}$$

then the associated transformation is

$$\begin{aligned} q' &= \partial_2 F_2(t, q, p') = q && (5.201)\\ p &= \partial_1 F_2(t, q, p') = p' - \partial_1 G(t, q) && (5.202)\\ H'(t, q', p') &= H(t, q, p) + \partial_0 F_2(t, q, p') \\ &= H(t, q, p) - \partial_0 G(t, q). && (5.203) \end{aligned}$$

Explicitly, the new Hamiltonian is

$$H'(t, q', p') = H(t, q', p' - \partial_1 G(t, q')) - \partial_0 G(t, q'), \tag{5.204}$$

where we have used the fact that $q = q'$. The transformation is interesting in that the coordinate transformation is the identity transformation, but the new and old momenta are not the same, even in the case in which G has no explicit time dependence. Suppose we have a Hamiltonian of the form

$$H(t, x, p) = \frac{p^2}{2m} + V(x) \tag{5.205}$$

then the transformed Hamiltonian is

$$H'(t, x', p') = \frac{(p' - \partial_1 G(t, x'))^2}{2m} + V(x') - \partial_0 G(t, x'). \tag{5.206}$$

We see that this transformation may be used to modify terms in the Hamiltonian that are linear in the momenta. Starting from H the transformation introduces linear momentum terms; starting from H' the transformation eliminates the linear terms.

We illustrate the use of this transformation with the driven pendulum. The Hamiltonian for the driven pendulum was derived automatically in section (3.1.1). We repeat the result here (cleaned up a bit)

$$\begin{aligned} &H(t, \theta, p_\theta) \\ &\quad = \frac{p_\theta^2}{2ml^2} - glm\cos\theta \\ &\qquad + gmy_s(t) - \frac{p_\theta}{l}\sin\theta Dy_s(t) - \frac{m}{2}(\cos\theta)^2(Dy_s(t))^2, \end{aligned} \tag{5.207}$$

where y_s is the drive function. The Hamiltonian is rather messy, and includes a term which is linear in the angular momentum with a coefficient that depends on both the angular coordinate and the time. Let's see what happens if we apply our transformation to the problem to eliminate the linear term. We can identify the transformation function G by requiring that the linear term in momentum is killed:

$$G(t, \theta) = -ml \cos\theta D y_s(t). \tag{5.208}$$

The transformed momentum is

$$p'_\theta = p_\theta + ml \sin\theta D y_s(t), \tag{5.209}$$

and the transformed Hamiltonian is

$$\begin{aligned} H'(t, \theta, p'_\theta) &= \frac{(p'_\theta)^2}{2ml^2} - ml(g + D^2 y_s)\cos\theta \\ &\quad + gmy_s(t) - \frac{m}{2}(y_s(t))^2 \end{aligned} \tag{5.210}$$

Dropping the last two terms, which do not affect the equations of motion, we find

$$H'(t, \theta, p'_\theta) = \frac{(p'_\theta)^2}{2ml^2} - ml(g + D^2 y_s)\cos\theta. \tag{5.211}$$

So we have found, by a straightforward canonical transformation, a Hamiltonian for the driven pendulum with the rather simple form of a pendulum with gravitational acceleration that is modified by the acceleration of the pivot. It is, in fact, the Hamiltonian that corresponds to the alternate form of the Lagrangian for the driven pendulum we found earlier by inspection (see equation 1.97). Here the derivation is by a simple canonical transformation, motivated by a desire to eliminate unwanted terms that are linear in the momentum.

5.4 Invariants of Canonical Transformations

Canonical transformations allow us to change the phase-space coordinate system that we use to express a problem, preserving the form of Hamilton's equations. If we solve Hamilton's equations in one phase-space coordinate system we can use the transformation to carry the solution to the other coordinate system. What other properties are preserved by a canonical transformation?

Noninvariance of pv

We noted in equation (5.10) that canonical extensions of point transformations preserved the value of pv. This does not hold for more general canonical transformations. We can illustrate this with the transformation just considered. Along corresponding paths x, p_x and θ, I

$$\begin{aligned} x(t) &= \sqrt{\frac{2I(t)}{\alpha}} \sin\theta(t) \\ p_x(t) &= \sqrt{2I(t)\alpha}\cos\theta(t). \end{aligned} \tag{5.212}$$

and so Dx is

$$Dx(t) = D\theta(t)\sqrt{\frac{2I(t)}{\alpha}}\cos\theta(t) + DI(t)\frac{1}{\sqrt{2I(t)\alpha}}\sin\theta(t). \tag{5.213}$$

So we can form

$$\begin{aligned} &p_x(t)Dx(t) - I(t)D\theta(t) \\ &\quad = I(t)D\theta(t)\left(2\cos^2\theta(t) - 1\right) + DI(t)\sin\theta(t)\cos\theta(t). \end{aligned} \tag{5.214}$$

In general this is not zero. The product pv is not necessarily invariant under general canonical transformations.

Invariance of Poisson Brackets

Here is a remarkable fact: the composition of the Poisson bracket of two phase space state functions with a canonical transformation is the same as the Poisson bracket of each of the two functions composed with the transformation separately. Loosely speaking, the Poisson bracket is invariant under canonical phase space transformations.

Let f and g be two phase space state functions. Using the $\widetilde{J}$ representation of the Poisson bracket (see section 5.2.4),

$$\begin{aligned} &\{f \circ C, g \circ C\}(s) \\ &\quad = (D(f\circ C))(s) \cdot (\widetilde{J} \circ D(g \circ C))(s) \\ &\quad = (Df \circ C)(s)) \cdot DC(s) \cdot (\widetilde{J} \circ ((Dg \circ C(s)) \cdot DC(s))) \\ &\quad = ((Df \circ C)(s)) \cdot \left(\Phi(DC(s)) \circ \widetilde{J} \circ \Phi^*(DC(s))\right)((Dg \circ C)(s)) \\ &\quad = ((Df \circ C)(s)) \cdot (\widetilde{J}((Dg \circ C)(s))) \\ &\quad = (\{f, g\} \circ C)(s), \end{aligned} \tag{5.215}$$

where the fact that C is symplectic and satisfies equation (5.31) was used in the middle. Abstracted to functions of phase-space states, this is:

$$\{f \circ C, g \circ C\} = \{f, g\} \circ C. \tag{5.216}$$

Volume Preservation

Consider a canonical transformation C. Let $\hat{C}_t$ be a function with parameter t such that $(q, p) = \hat{C}_t(q', p')$ if $(t, q, p) = C(t, q', p')$. The function $\hat{C}_t$ maps phase space coordinates to alternate phase space coordinates at a given time. Consider regions R in (q, p) and R' in (q', p') such that $R = \hat{C}_t(R')$. The volume of region R' is

$$V(R) = \int_R 1 = \int_{R'} \det(D\hat{C}_t) \tag{5.217}$$

Now if C is symplectic then the determinant of $D\hat{C}_t$ is one (see section 4.2), so

$$V(R) = V(R'). \tag{5.218}$$

Thus, phase space volume is preserved by symplectic transformations.

Liouville's theorem shows that time evolution preserves phase space volume. Here we see that canonical transformations also preserve phase volumes. Later, we will find that time evolution actually generates a canonical transformation.

A bilinear form preserved by symplectic transformations

The invariance of Poisson brackets under canonical transformations can be used to prove the invariance of another closely-related antisymmetric bilinear form under canonical transformations. Define[19]

$$\omega(\zeta_1, \zeta_2) = P(\zeta_2)Q(\zeta_1) - P(\zeta_1)Q(\zeta_2), \tag{5.219}$$

[19] The ω form can also be written as a sum over degrees of freedom:

$$\omega(\zeta_1, \zeta_2) = \sum_i P_i(\zeta_2)Q^i(\zeta_1) - P_i(\zeta_1)Q^i(\zeta_2).$$

Notice that the contributions for each i do not mix components from different degrees of freedom.

where Q and P are the coordinate and momentum selectors, respectively. The arguments ζ_1 and ζ_2 are incremental phase space states. Under a canonical transformation $s = C(s')$, incremental states transform with the derivative

$$\zeta_i = DC(s')\zeta'_i. \tag{5.220}$$

We will show that

$$\omega(\zeta_1, \zeta_2) = \omega(\zeta'_1, \zeta'_2), \tag{5.221}$$

provided the ζ_i have zero time component.

We have found that the symplectic condition (5.27) for Hamiltonians that transform by composition depends only on C and not on the Hamiltonian. Thus if we have a canonical transformation, the symplectic condition is satisfied for any real valued function f on the phase state space:

$$\widetilde{J}(Df(C(s))) = DC(s) \cdot \widetilde{J}((D(f \circ C))(s)). \tag{5.222}$$

We will use this in the following.

We can write the Poisson bracket in terms of ω:

$$\{f, g\}(s) = \omega((\tilde{J} \circ Df)(s), (\tilde{J} \circ Dg)(s)), \tag{5.223}$$

as can be seen by writing out the components. We use the fact that Poisson brackets are invariant under canonical transformations

$$(\{f, g\} \circ C)(s') = \{f \circ C, g \circ C\}(s'). \tag{5.224}$$

The left hand side of equation (5.224) is

$$\begin{aligned} (\{f, g\} \circ C)(s') &= \omega((\tilde{J} \circ Df \circ C)(s'), (\tilde{J} \circ Dg \circ C)(s')) \\ &= \omega(DC(s') \cdot (\tilde{J} \circ (D(f \circ C)(s'))), \\ &\qquad DC(s') \cdot (\tilde{J} \circ (D(g \circ C)(s')))), \end{aligned} \tag{5.225}$$

where we have used the useful relation (5.222). The right-hand side of equation (5.224) is

$$\{f \circ C, g \circ C\}(s') = \omega((\tilde{J} \circ D(f \circ C))(s'), (\tilde{J} \circ D(g \circ C))(s')). \tag{5.226}$$

Now the left-hand side must equal the right hand side for any f and g, so the equation must also be true for arbitrary ζ_i of the form:

$$\begin{aligned}\zeta_1' &= (\tilde{J} \circ D(f \circ C))(s') \\ \zeta_2' &= (\tilde{J} \circ D(g \circ C))(s').\end{aligned} \tag{5.227}$$

The ζ_i' are arbitrary incremental states with zero time components.

So we have proven that

$$\omega(\zeta_1', \zeta_2') = \omega(DC(s') \cdot \zeta_1',\, DC(s') \cdot \zeta_2'). \tag{5.228}$$

for canonical C and incremental states ζ_i with zero time components. Using equation (5.220) we have

$$\omega(\zeta_1', \zeta_2') = \omega(\zeta_1, \zeta_2). \tag{5.229}$$

Thus the bilinear antisymmetric function ω is invariant under canonical transformations.

As a program ω is:

```
(define (omega zeta1 zeta2)
  (- (* (momentum zeta2) (coordinate zeta1))
     (* (momentum zeta1) (coordinate zeta2))))
```

We can check that it is invariant under the polar to rectangular canonical transformation by computing the residuals. We use the arbitrary state

```
(define a-polar-state
  (->H-state 't
             (coordinate-tuple 'r 'varphi)
             (momentum-tuple 'p_r 'p_varphi)))
```

and the typical state increments

```
(define zeta1
  (->H-state 0
             (typical-object (coordinate a-polar-state))
             (typical-object (momentum a-polar-state))))

(define zeta2
  (->H-state 0
             (typical-object (coordinate a-polar-state))
             (typical-object (momentum a-polar-state))))
```

Note the time components of `zeta1` and `zeta2` are zero. We evaluate the residual:

```
(let ((DCs ((D (F->CT p->r)) a-polar-state)))
  (pe (- (omega zeta1 zeta2)
         (omega (* DCs zeta1) (* DCs zeta2)))))
0
```

The residual is zero so ω is invariant under this canonical transformation.

Poincaré Integral Invariants

Consider the oriented area of a region R' in phase space (see figure 5.7). Suppose we make a canonical transformation from coordinates (q', p') to (q, p) taking region R' to region R. The boundary of the region in the transformed coordinates is just the image under the canonical transformation of the original boundary. The image of a planar region is not necessarily planar, but even if it is it need not have the same area as the original region. Let R_{q^i,p_i} be the projection of the region R onto the q^i, p_i plane of coordinate q^i and conjugate momentum p_i, and A_i be its area. We call the q^i, p_i plane the i^{th} *canonical plane* in these phase space variables. Similarly, let $R'_{q'^i,p'_i}$ be the projection of R' onto the q'^i, p'_i plane, and A'_i be its area. Then it turns out that the sum of the areas of the projections of R and R' are the same:

$$\sum_i A_i = \sum_i A'_i. \tag{5.230}$$

That is, the sum of the projected areas on the canonical planes is preserved by canonical transformations. Another way to say this is

$$\sum_i \int_{R_{q^i,p_i}} dq^i dp_i = \sum_i \int_{R'_{q'^i,p'_i}} dq'^i dp'_i. \tag{5.231}$$

That's pretty interesting and pretty weird.

To see why this is true we first consider how the area of an incremental parallelogram in phase space transforms under canonical transformation. Let $(\Delta q, \Delta p)$ and $(\delta q, \delta p)$ represent small increments in phase space, originating at (q, p). Consider the incremental parallelogram with vertex at (q, p) with these two phase

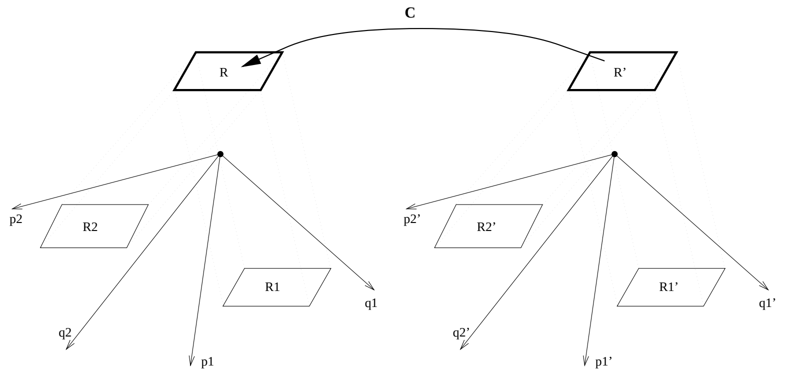

Figure 5.7 A region R' in phase space is mapped by a canonical tranformation C to a region R. The projections of region R onto the planes formed by canonical basis pairs (q_j, p_j) are R_j. The projections of R' are R'_j. In general, the areas of the regions R and R' are not the same, but the sum of the areas of the canonical plane projections are the same.

space increments as edges. The sum of the areas of the canonical projections of this incremental parallelogram can be written

$$\sum_i \Delta A_i = \sum_i (\Delta q^i \delta p_i - \Delta p_i \delta q^i). \tag{5.232}$$

The right hand side is the sum of the areas on the canonical planes; for each i we see the area of a parallelogram computed from the components of the vectors defining its adjacent sides. Let $\zeta_1 = (0, \Delta q, \Delta p)$ and $\zeta_2 = (0, \delta q, \delta p)$, then the sum of the areas of the incremental parallelograms is just

$$\sum_i \Delta A_i = \omega(\zeta_1, \zeta_2), \tag{5.233}$$

where ω is the bilinear antisymmetric function introduced above. The function ω is invariant under canonical transformations, so the sum of the areas of the incremental parallelograms is invariant under canonical transformations.

The area of an arbitrary region is just the limit of the sum of the areas of incremental parallelograms that cover the region, so the sum of oriented areas is preserved by canonical transformations:

$$\sum_i A_i = \sum_i A'_i. \tag{5.234}$$

We define an *action-like region* to be one for which canonical coordinates can be chosen so that the region is entirely in the subspace spanned by a particular canonical pair (q^i, p_i). For this coordinate system the projection on that plane has all of the area. The projections on the other canonical planes have no area. So the sum of the areas of the canonical projections is just the area of the region itself. The sum of the areas of the projections onto canonical planes is preserved under canonical transformation so the area of an action-like region is the sum of the areas of the canonical projections for any canonical coordinate system.

There are also regions which have no action-like projection. For example, a region in the plane (q^i, q^j) has no action-like projection. Therefore the sum of the areas of the canonical projections is zero, and this is the case for any canonical coordinate system, though in other canonical coordinates some of the projections may have non-zero area to be balanced by negative area of others.

5.5 Origin of Generating Functions

Generating functions can be used to specify a canonical transformation by the prescription given above. We have shown that this prescription gives a canonical transformation. However, we have given no derivation of the rules. Where did they come from? The following is an incorrect derivation of these rules for the generating function. As you read it try to find the bug.

An Incorrect Derivation

Let L and L' be the Lagrangians expressed in two coordinate systems for which the path is q and q', respectively. We further assume that the value of L and L' on the path differ by the time derivative of a function of the configuration and time evaluated on the path. This function can be written in terms of the path expressed in terms of both sets of coordinates. Consider the function $F_1(t, q, q')$, and its value on the path $\widetilde{F}_1(t) = F_1(t, q(t), q'(t))$

at time t. The time derivative of $\widetilde{F}_1$ is

$$\begin{aligned} D\widetilde{F}_1(t) &= (\partial_1 F_1)(t, q(t), q'(t))Dq(t) \\ &\quad + (\partial_2 F_1)(t, q(t), q'(t))Dq'(t) \\ &\quad + \partial_0 F_1(t, q(t), q'(t)). \end{aligned} \tag{5.235}$$

The relation between the Lagrangians is therefore

$$\begin{aligned} &L(t, q, \dot{q}) - L'(t, q', \dot{q}') \\ &\quad = (\partial_1 F_1)(t, q, q')\dot{q} + (\partial_2 F_1)(t, q, q')\dot{q}' + \partial_0 F_1(t, q, q'). \end{aligned} \tag{5.236}$$

Now rewrite the Lagrangians in terms of the Hamiltonians

$$\begin{aligned} &[p\dot{q} - H(t, q, p)] - [p'\dot{q}' - H'(t, q', p')] \\ &\quad = \partial_1 F_1(t, q, q')\dot{q} + \partial_2 F_1(t, q, q')\dot{q}' + \partial_0 F_1(t, q, q'), \end{aligned} \tag{5.237}$$

where p is determined by t, q, and $\dot{q}$ and the Lagrangian L. Similar relations hold for the primed functions. Let's collect terms

$$\begin{aligned} 0 &= [p - \partial_1 F_1(t, q, q')]\dot{q} \\ &\quad - [p' + \partial_2 F_1(t, q, q')]\dot{q}' \\ &\quad - H(t, q, p) + H'(t, q', p') - \partial_0 F_1(t, q, q'). \end{aligned} \tag{5.238}$$

If the relations (5.64–5.66) hold then each of these lines is independently zero, apparently verifying that the Lagrangians differ by a total time derivative. If this were true then the equations of motion would be preserved and the transformation would have been shown to be canonical.[20]

What's wrong?

So what is wrong with this derivation? Let's consider a specific example and calculate all the details.

[20] Many texts further muddy the matter by introducing an unjustified independence argument here: they argue that because $\dot{q}$ and $\dot{q}'$ are independent the relations (5.64–5.66) must hold. This is silly, because p and p' are functions of $\dot{q}$ and $\dot{q}'$, respectively, so there are implied dependencies of the velocities in many places, so it is unjustified to separately set pieces of this equation to zero. However, notwithstanding this problem, the derivation of the fact that the transformation is canonical is fallacious, as we will see.

Consider the simple Lagrangian

$$L(t, x, \dot{x}) = \frac{1}{2}\dot{x}^2 - \frac{1}{4}x^4. \tag{5.239}$$

The momentum is $p_x = \partial_2 L(t, x, \dot{x}) = \dot{x}$, and the Hamiltonian is

$$H(t, q, p_x) = p_x \dot{x} - L(t, x, \dot{x}) = \frac{1}{2}p_x^2 + \frac{1}{4}x^4. \tag{5.240}$$

The equation of motion is

$$D^2 x = D p_x = -x^3. \tag{5.241}$$

Now consider a simple canonical transformation from (x, p_x) to (y, p_y) generated by

$$F_1(t, x, y) = xy, \tag{5.242}$$

with associated equations

$$p_x = \partial_1 F_1(t, x, y) = y \tag{5.243}$$

$$p_y = -\partial_2 F_1(t, x, y) = -x \tag{5.244}$$

$$H'(t, y, p_y) = H(t, x, p_x). \tag{5.245}$$

This transformation just interchanges the coordinate and momentum. So the transformed Hamiltonian is

$$H'(t, y, p_y) = \frac{1}{2}y^2 + \frac{1}{4}p_y^4. \tag{5.246}$$

It is easy to check that the transformation is canonical by computing the fundamental Poisson bracket $\{y, p_y\} = \{p_x, -x\} = \{x, p_x\} = 1$ (with $H = H'$). Hamilton's equations are

$$D p_y = -y \tag{5.247}$$

$$D y = p_y^3 \tag{5.248}$$

Given the relation $x = p_y$ these are obviously equivalent to the original equations of motion.

Next we compute the Lagrangian associated with this Hamiltonian through a Legendre transform. We have

$$D y = \partial_2 H'(t, y, p_y) = p_y^3, \tag{5.249}$$

and

$$L'(t, y, \dot{y}) = p_y \dot{y} - H(t, y, p_y) = \frac{3}{4}\dot{y}^{4/3} - \frac{1}{2}y^2. \tag{5.250}$$

The Lagrange equations are

$$D^2 y = -3(Dy)^{2/3} y. \tag{5.251}$$

We can check that this is equivalent to the original Lagrange equation by differentiating the original equation to get

$$D^3 x = -3x^2 Dx \tag{5.252}$$

Then using the relations $Dx = p_x = y$ and $x = -p_y = -(Dy)^{1/3}$ we derive

$$D^2 y = -3(Dy)^{2/3} y, \tag{5.253}$$

which is the same as the Lagrange equation.

Now consider the difference between the two Lagrangians. We calculate

$$\Delta L = L - L' = \frac{1}{2}\dot{x}^2 - \frac{1}{4}x^4 - \frac{3}{4}\dot{y}^{4/3} + \frac{1}{2}y^2. \tag{5.254}$$

Expressed in terms of x and $\dot{x}$ this is

$$\Delta L = \dot{x}^2 - x^4. \tag{5.255}$$

Here is the surprise. The difference of the two Lagrangians is not a total time derivative, as was assumed in the derivation of the generating functions. Thus the generating function method is not justified by the freedom to add total time derivatives to Lagrangians.

However, using $p_x = \dot{x}$, which on path is $p_x = Dx$, and the equation of motion, $Dp_x = -x^3$, we can reexpress the difference of Lagrangians as

$$\Delta L = p_x Dx + Dp_x x = D(xp_x). \tag{5.256}$$

So with the help of the equations of motion we can represent the difference of the Lagrangians as the total time derivative of a phase space function $F(x, p_x) = xp_x$. Only on a solution trajectory is the difference a total time derivative.

The derivation that was presented of the generating function relations for a canonical transformation is wrong. Starting with the generating function relations the derivation seemed to show that the two Lagrangians differed by a total time derivative and thus were equivalent. However, direct calculation showed that what looked like a total time derivative was in fact only a total time derivative along solution trajectories.

5.5.1 Generating Functions and Integral Invariants

The generating function representation of canonical transformations can be derived from the Poincaré integral invariants. The outline is the following. We first show that, given a canonical transformation, the integral invariants imply the existence of a function of phase-space coordinates that can be written as a path-independent line integral. Then we show that partial derivatives of this function, represented in mixed coordinates, give the generating function relations between the old and new coordinates. We only need to do this for time independent transformations because time dependent transformations become time independent in the extended phase space.

Recall the result about integral invariants from Section 5.4. There we found that

$$\oint_{\partial R} \sum p_i dq^i = \oint_{\partial R'} \sum p'_i dq'^i, \tag{5.257}$$

where R' is a two dimensional region in (q', p') coordinates at time t, and $R = C(t, R')$ is the corresponding region in (q, p) coordinates, and where ∂R indicates the boundary of the region R. This holds for any region and its boundary. We shall show that this implies there is a function $F(t, q', p')$, which can be defined in terms of these line integrals

$$F(t, q', p') - F(t, q'_0, p'_0) = \int_{C(t,\gamma')} \sum p_i dq^i - \int_{\gamma'} \sum p'_i dq'^i, \tag{5.258}$$

where γ' is a curve in phase space coordinates that begins at (q'_0, p'_0) and ends at (q', p'). We can show that the value of F does not depend on the intermediate path by computing the difference of F along one path γ_1 between the specified endpoints and comparing it to the value of F computed along a different path γ_2 with the same endpoints. The difference between these values can be written as a difference of integrals around loops from (q'_0, p'_0) to (q', p') and back again to (q'_0, p'_0)

$$\begin{aligned}(F_{\gamma_1}(t, q', p') - F_{\gamma_1}(t, q'_0, p'_0)) &- (F_{\gamma_2}(t, q', p') - F_{\gamma_2}(t, q'_0, p'_0)) \\ &= \oint_{\partial R} \sum p_i dq^i - \oint_{\partial R'} \sum p'_i dq'^i \\ &= 0 \end{aligned} \tag{5.259}$$

where here R is the region enclosed by the two paths, and the result is zero because of the integral invariant equation (5.257). So we conclude that F has a well-defined value that is independent of the path taken to compute it.

The phase-space point (q, p) in unprimed variables corresponds to (q', p') in primed variables, at an arbitrary time t. Both p and q are determined given q' and p'. In general, given any two of these four quantities we can solve for the other two. We can introduce functions

$$\begin{aligned} p &= f_p(t, q, q') \\ p' &= f_{p'}(t, q, q') \end{aligned} \tag{5.260}$$

that solve the transformation equations $(t, q, p) = C(t, q', p')$ for the momenta in terms of the coordinates at a specified time. With these we can introduce a function $F_1(t, q, q')$ such that

$$F_1(t, q, q') = F(t, q, f_p(t, q, q')). \tag{5.261}$$

The function F_1 has the same value as F but has different arguments. We shall show that this F_1 is in fact the generating function for canonical transformations introduced in section 5.3. Let's be explicit about the definition of F_1 in terms of a line integral

$$\begin{aligned} &F_1(t, q, q') - F_1(t, q_0, q'_0) \\ &\quad = \int_{q_0, q'_0}^{q, q'} (f_p(t, q, q')dq - f_{p'}(t, q, q')dq'). \end{aligned} \tag{5.262}$$

The two line integrals can be combined into this one because they are both expressed as integrals along a curve in (q, q').

We can use the path independence of F_1 to compute the partial derivatives of F_1 with respect to particular components and consequently derive the generating function relations for the momenta. Let's recall what we mean by a partial derivative of F_1 with respect to one of the components of q, say q^i. To do this we introduce a function

$$\begin{aligned}
&\Delta F_1(t, q, q')(\Delta q^i) \\
&\quad = F_1(t; q_1, \ldots, q^i + \Delta q^i, \ldots, q^n; q'^1, \ldots, q'^n) \\
&\qquad - F_1(t; q_1, \ldots, q^i, \ldots, q^n; q'^1, \ldots, q'^n).
\end{aligned} \tag{5.263}$$

The partial derivative of F_1 with respect to the i^{th} component of the q argument, is the derivative of $\Delta F_1(t, q, q')$

$$(\partial_1 F_1(t, q, q'))^i = D(\Delta F_1(t, q, q'))(0). \tag{5.264}$$

The function F_1 is defined as a path independent line integral; so we can compute ΔF_1 as a line integral along the increment Δq^i

$$\begin{aligned}
&\Delta F_1(t, q, q')(\Delta q^i) \\
&\quad = \int_{q,q'}^{q+\Delta q^i, q'} \left(\sum_j f_{p_j}(t, q, q') dq^j - \sum_j f_{p'_j}(t, q, q') dq'^j \right),
\end{aligned} \tag{5.265}$$

but this is the same as

$$\Delta F_1(t, q, q')(\Delta q^i) = \int_{q,q'}^{q+\Delta q^i, q'} f_{p_i}(t, q, q') dq^i \tag{5.266}$$

because the line of integration is an increment along a single component direction. However, this is now an ordinary integral so we can use the fundamental theorem of calculus to give us the derivative

$$(\partial_1 F_1(t, q, q'))^i = D(\Delta F_1(t, q, q'))(0) = f_{p_i}(t, q, q'). \tag{5.267}$$

A similar argument shows that

$$(\partial_2 F_1(t, q, q'))^i = -f_{p'_i}(t, q, q'). \tag{5.268}$$

These are just the configuration and momentum parts of the generating function relations for canonical transformation. So starting with a canonical transformation, we can find a generating function that gives the coordinate-momentum part of the transformation through its derivatives.

Starting from a general canonical transformation, we have constructed an F_1 generating function from which the canonical transformation may be rederived. So, we expect there is a generating function for every canonical transformation.[21]

5.6 Extended Phase Space

In this section we explore the significance of time, and find that it has none. We find that we can treat time as just another coordinate if we wish. Systems described by a time-dependent Hamiltonian may be recast in terms of a time-independent Hamiltonian with an extra degree of freedom. An advantage of this view is that what was a time-dependent canonical transformation can be treated as a time-independent transformation, where there are no additional conditions for adjusting the Hamiltonian.

Consider a dynamical system with n degrees of freedom, whose behavior is described by a time-dependent Hamiltonian $H(t, q, p)$. We construct the *extended phase space* as follows: introduce a new set of coordinates that are the same as the old coordinates except that there is one additional coordinate t, the time. Similarly, define a new set of momenta that are the same as the old momenta except for an additional momentum T conjugate to time. Finally, introduce a new independent variable τ. The idea is to define a Hamiltonian in the extended phase space $H_e(\tau; q, t; p, T)$ so that $t(\tau) = \tau$, so the extra time coordinate has the same value as the independent variable τ. For this to work out we need $Dt(\tau) = 1$, for then (with suitable initial conditions) $t(\tau) = \tau$. The Hamilton's equation that governs the evolution of t is

$$Dt(\tau) = (\partial_2 H_e)^n(\tau; q, t; p, T) = 1. \tag{5.269}$$

We may achieve this by choosing

$$H_e(\tau; q, t; p, T) = T + \cdots. \tag{5.270}$$

[21] There may be some singular cases and topological problems that prevent this from being rigorously true.

We want the original Hamilton's equations for q and p to be unmodified so the extended phase space Hamiltonian can be taken to be

$$H_e(\tau; q, t; p, T) = T + H(t, q, p). \tag{5.271}$$

With this choice the time coordinate t maintains the same value as the independent variable τ, and the other Hamilton's equations are unmodified.

More formally, consider Hamilton's equations for q in the extended phase space

$$\begin{aligned}
&Dq^i(\tau) \\
&\quad = (\partial_2 H_e)^i(\tau; q^0(\tau), \cdots, q^{n-1}(\tau), t(\tau); \\
&\qquad\qquad p_0(\tau), \cdots, p_{n-1}(\tau), T(\tau)) \\
&\quad = (\partial_2 H)^i(\tau; q^0(\tau), \cdots, q^{n-1}(\tau); p_0(\tau), \cdots, p_{n-1}(\tau)),
\end{aligned} \tag{5.272}$$

but this is just the usual Hamilton's equation for q^i with a different name for the independent variable. A similar argument shows the Hamilton's equations for p in the extended phase space are the same as the original Hamilton's equations.

Notice that the Hamiltonian in the extended phase space does not depend on the independent variable, whether or not the original Hamiltonian depends on the original independent variable time. Thus the extended Hamiltonian is a conserved quantity. Its value is constant along realizable paths. The value of the original Hamiltonian is the energy, E, whether or not it is conserved. The value of the extended Hamiltonian is the sum of the value of T and the energy, so the value of the momentum T is, up to an additive constant, minus the energy.

Hamilton's equation for T is

$$\begin{aligned}
&DT(\tau) \\
&\quad = -(\partial_1 H_e)_n(\tau; q^0(\tau), \cdots, q^{n-1}(\tau), t(\tau); \\
&\qquad\qquad p_0(\tau), \cdots, p_{n-1}(\tau), T(\tau)) \\
&\quad = -\partial_0 H(\tau, q(\tau), p(\tau)).
\end{aligned} \tag{5.273}$$

We know that

$$DE(t) = \partial_0 H(t, q(t), p(t)), \tag{5.274}$$

so

$$DT(\tau) = -DE(\tau). \tag{5.275}$$

Thus

$$T(\tau) = E_0 - E(\tau). \tag{5.276}$$

The constant E_0 has no dynamical significance, so we can choose it to be zero. Having made this choice we now can say, "The momentum conjugate to time is the negative of the total energy of the system."

Note that the extension transformation is canonical in the sense that the two sets of equations of motion describe equivalent dynamics. However, the transformation is not symplectic.

Restricted Three-Body Problem

An example that shows the utility of reformulating a problem in the extended phase space is the restricted three-body problem: the motion of a low mass particle subject to the gravitational attraction of two other massive bodies, which move in some fixed orbit. The problem is an idealization of the situation where a body with very small mass moves in the presence of two bodies with much larger masses. The motion of the larger bodies is presumed not to be influenced by the motion of the smaller body. In the simplest version, the motion of all three bodies is assumed to be in the same plane, and the orbit of the two massive bodies is circular.

Because the motion of the bodies with larger masses is not influenced by the small mass we model this situation as the small body moving in a time-varying field of the larger bodies undergoing a prescribed motion. This situation can be captured as a time dependent Hamiltonian:

$$H(t; x, y; p_x, p_y) = \frac{p_x^2 + p_y^2}{2m} - \frac{Gmm_1}{r_1} - \frac{Gmm_2}{r_2} \tag{5.277}$$

where r_1 and r_2 are the distances of the small body to the larger bodies, and where m is the mass of the small body, and m_1 and m_2 are the masses of the larger bodies. Note that r_1 and r_2 are quantities that depend both on the position of the small particle and the time-varying position of the massive particles.

The massive bodies are in circular orbits, and maintain constant distance from the center of mass. Let a_1 and a_2 be the distances to the center of mass, then the distances satisfy $m_1 a_1 = m_2 a_2$. The angular frequency is $\Omega = \sqrt{G(m_1 + m_2)/a^3}$ where a is the distance between the masses.

In polar coordinates, with the center of mass of the subsystem of massive particles at the origin, and with r and θ describing the position of the low-mass particle, the positions of the two massive bodies are $a_2 = m_1 a/(m_1+m_2)$ with $\theta_2 = \Omega t$, $a_1 = m_2 a/(m_1+m_2)$ with $\theta_1 = \Omega t + \pi$. The distances to the point masses are

$$\begin{aligned} r_2^2 &= r^2 + a_2^2 - 2a_2 r \cos(\theta - \Omega t) \\ r_1^2 &= r^2 + a_1^2 - 2a_1 r \cos(\theta - \Omega t - \pi). \end{aligned} \tag{5.278}$$

So, in polar coordinates, the Hamiltonian is

$$H(t; r, \theta; p_r, p_\theta) = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2}\right) - \frac{Gmm_1}{r_1} - \frac{Gmm_2}{r_2}. \tag{5.279}$$

We see therefore that the Hamiltonian can be written in terms of some function f such that

$$H(t; r, \theta; p_r, p_\theta) = f(r, \theta - \Omega t, p_r, p_\theta). \tag{5.280}$$

The essential feature is that θ and t only appear in the Hamiltonian in the combination $\theta - \Omega t$.

One way to get rid of the time dependence, is to choose a new set of variables with one coordinate equal to this combination $\theta - \Omega t$, by making a point transformation to a rotating frame. We have shown that

$$r' = r \tag{5.281}$$

$$\theta' = \theta - \Omega t \tag{5.282}$$

$$p_r' = p_r \tag{5.283}$$

$$p_\theta' = p_\theta \tag{5.284}$$

with

$$\begin{aligned} H'(t; r', \theta'; p_r', p_\theta') &= H(t; r', \theta' + \Omega t; p_r', p_\theta') - \Omega p_\theta' \\ &= f(r', \theta', p_r', p_\theta') - \Omega p_\theta' \end{aligned} \tag{5.285}$$

is a canonical transformation. The new Hamiltonian is not the energy but it is conserved. It is a useful integral of motion—the Jacobi constant.[22]

We can also eliminate the dependence on the independent time-like variable from the Hamiltonian for the restricted problem by going to the extended phase space. The Hamiltonian

$$\begin{aligned} H_e(\tau; r, \theta, t; p_r, p_\theta, T) &= H(t; r, \theta; p_r, p_\theta) + T \\ &= f(r, \theta - \Omega t, p_r, p_\theta) + T \end{aligned} \tag{5.286}$$

is autonomous and is consequently an integral of the motion. Again, we see that θ and t only occur in the combination $\theta - \Omega t$, which suggests a point transformation to a new coordinate $\theta' = \theta - \Omega t$. This point transformation is independent of the new independent variable τ. We can work out the details using an F_2 generating function:

$$F_2(\tau; r, \theta, t; p_r', p_\theta', T') = r p_r' + (\theta - \Omega t) p_\theta' + t T' \tag{5.287}$$

which gives the same transformation as specified in equations (5.281–5.284) plus

$$t' = t \tag{5.288}$$

$$T = -\Omega p_\theta' + T', \tag{5.289}$$

with the new Hamiltonian obtained by composing the old Hamiltonian with the transformation (no $\partial F / \partial t$ term!)

$$\begin{aligned} &H_e'(\tau; r', \theta', t'; p_r', p_\theta', T') \\ &\quad = H_e(\tau; r', \theta' + \Omega t', t'; p_r', p_\theta', T' - \Omega p_\theta') \\ &\quad = f(r', \theta', p_r', p_\theta') + T' - \Omega p_\theta' \end{aligned} \tag{5.290}$$

We recognize that the new Hamiltonian in the extended phase space, which has the same value as the original Hamiltonian in the extended phase space, is just the Jacobi constant plus T'. Now, the new Hamiltonian does not depend on t' so T' is a constant of the motion. In fact its value is irrelevant to the rest of the dynamical evolution, so we may set the value of T' to zero if we like. Thus, we have found that the Hamiltonian in the extended

[22] Actually, the traditional Jacobi constant is $C = -2H'$.

phase space, which is conserved, is just the Jacobi constant plus an additive arbitrary constant. We have two routes to the Jacobi constant: (1) transform the original system to a rotating frame to eliminate the time dependence, but in the process add extra terms to the Hamiltonian arising from the time dependence of th generating function, and (2) go to the extended phase space and immediately get an integral, and by going to a rotating frame of reference recognize that this Hamiltonian is the same as the Jacobi constant. So sometimes the Hamiltonian in the extended phase space is a useful integral.

5.6.1 Transformations in the Extended Phase Space

In section 5.2.3 we found that time-dependent transformations for which the derivative of the coordinate-momentum part is symplectic are canonical only if the Hamiltonian is modified by adding a function K subject to certain constraints. In this section we show that the constraints on K follow from the symplectic condition in the extended phase space.

Recall that the following specifies a time dependent canonical transformation

$$\begin{aligned} q &= A(t, q', p') \\ p &= B(t, q', p') \\ H'(t, q', p') &= H(t, A(t, q', p'), B(t, q', p')) + K(t, q', p'), \end{aligned} \tag{5.291}$$

if A and B satisfy the fundamental Poisson bracket relations, and if K satisfies

$$\begin{aligned} 0 &= \partial_0 A + \{A, K\} \\ 0 &= \partial_0 B + \{B, K\}. \end{aligned} \tag{5.292}$$

Let's rewrite this as an extended phase space transformation. The Hamiltonian in the extended phase space is

$$H_e(\tau; q, t; p, T) = H(t, q, p) + T, \tag{5.293}$$

where we have left q, p, t, and T as separate variables though in the extended phase space we consider t to be one of the coordinates, and T to be one of the momenta. The transformed Hamiltonian in the extended phase space is

$$H'_e(\tau; q', t'; p', T') = H'(t', q', p') + T'. \tag{5.294}$$

Using the expression for H' in terms of H and K

$$\begin{aligned} &H'_e(\tau; t', q'; T', p') \\ &\quad = H'(t', q', p') + T' \\ &\quad = H(t', A(t', q', p'), B(t', q', p')) + T' + K(t', q', p') \\ &\quad = H_e(\tau; A(t', q', p'), t'; B(t', q', p'), T' + K(t', q', p')). \end{aligned} \tag{5.295}$$

We see that the extended Hamiltonians transform by composition $H'_e = H_e \circ C_e$ if the extended phase space transform is

$$\begin{pmatrix} \tau \\ q \\ t \\ p \\ T \end{pmatrix} = C_e \begin{pmatrix} \tau \\ q' \\ t' \\ p' \\ T' \end{pmatrix} = \begin{pmatrix} \tau \\ A(t', q', p') \\ t' \\ B(t', q', p') \\ T' + K(t', q', p') \end{pmatrix}. \tag{5.296}$$

The Hamiltonians in the extended phase space transform by composition and the extended transformation does not depend upon the new time-like variable, so the transformation is canonical if the extended qp part of DC_e is symplectic. We will show that this is equivalent to the symplectic condition on the original qp part of the transformation plus the additional constraint equations on K.

The symplectic condition is equivalent to the fundamental Poisson bracket conditions. Here the Poisson brackets are in the extended phase space, so we need to understand the relationship of the Poisson brackets in the original phase space to those in the extended phase space. Let f_e and g_e be functions of the extended phase space tuple $(\tau; q, t; p, T)$. The extended Poisson bracket of f_e and g_e is

$$\begin{aligned} \{f_e, g_e\}_e &= \sum_{i=0}^{n} \left((\partial_1 f_e)_i (\partial_2 g_e)^i - (\partial_2 f_e)^i (\partial_1 g_e)_i \right) \\ &= \{f_e, g_e\} + (\partial_1 f_e)_0 (\partial_2 g_e)^0 - (\partial_2 f_e)^0 (\partial_1 g_e)_0 \end{aligned} \tag{5.297}$$

where the usual Poisson bracket on extended phase space functions is computed by summing over the usual coordinates and momenta $0 \le i \le n-1$. The additional terms contain derivatives with respect to the t and T variables. Now if f_e and g_e do not depend explicitly on T then the value of the extended Poisson bracket is the same as the value of the unextended Poisson bracket—the additional terms are zero.

The Poisson brackets of the components of C_e that give the usual coordinates and momenta reduce to the usual Poisson brackets of the coordinates and momenta

$$\begin{aligned}
\{(C_e)^q, (C_e)^p\}_e &= \{A, B\} \\
\{(C_e)^q, (C_e)^q\}_e &= \{A, A\} \\
\{(C_e)^p, (C_e)^p\}_e &= \{B, B\}.
\end{aligned} \tag{5.298}$$

These are the fundamental Poisson brackets for the original unextended transformation. The Poisson bracket of the t component of C_e with the other components are zero except for the T component. There the Poisson bracket of t with the K part is zero because K does not depend on T. We are left with

$$\{(C_e)^t, (C_e)^T\}_e = 1. \tag{5.299}$$

This confirms that t and T are conjugate variables. The Poisson brackets of the ordinary coordinate and momentum part of C_e with the T component of C_e are

$$\begin{aligned}
\{(C_e)^q, (C_e)^T\}_e &= \partial_0 A + \{A, K\} \\
\{(C_e)^p, (C_e)^T\}_e &= \partial_0 B + \{B, K\}.
\end{aligned} \tag{5.300}$$

These are the conditions on K that are required so that the transformation is canonical.

Earlier we found that time-dependent transformations are canonical if the qp part of the transformation is symplectic, and the Hamiltonian transforms by composition plus a correction. In the extended phase space, what were time-dependent transformations are independent of the new independent variable. Now we see that if the Hamiltonians in the extended phase space transform by composition and the qp part of the extended transformation is symplectic then the transformation is canonical. The test for symplectic in the extended phase space is equivalent to the symplectic plus Hamiltonian correction conditions in the original unextended phase space.

We can represent canonical transformations with mixed variable generating functions. We can extend these to represent transformations in the extended phase space. Let F_2 be a generating function with arguments (t, q, p'). Then, the corresponding F_2^e in the extended phase space can be taken to be

$$F_2^e(\tau; q, t; p', T') = tT' + F_2(t, q, p). \tag{5.301}$$

The relations between the coordinates and the momenta are the same as before. We also have

$$\begin{aligned} T &= (\partial_1 F_2^e)_n(\tau; q, t; p', T') = T' + \partial_0 F_2(t, q, p) \\ t' &= (\partial_2 F_2^e)^n(\tau; q, t; p', T') = t. \end{aligned} \tag{5.302}$$

The first equation gives the relationship between the original Hamiltonians:

$$H'(t, q', p') = H(t, q, p) + \partial_0 F_2(t, q, p), \tag{5.303}$$

as required. We know that time-independent canonical transformations have symplectic qp part. The generating function representation of a time dependent transformation does not depend on the independent variable in the extedned phase space, and so has symplectic qp part. That the generating function in the extended phase space gives the same transformation in the original phase space thus shows that the qp part is symplectic even if the generating function is time-dependent. Thus all canonical transformations generated by generating functions have symplectic qp part, whether or not they are time-dependent.

5.6.2 Poincaré-Cartan Integral Invariant

A time-dependent transformation is canonical if in the extended phase space the Hamiltonians transform by composition and the extended phase space transformation is symplectic. In Section 5.4 we have shown that if the derivative of the transformation is symplectic then the sum of the areas of the projections of any two-dimensional region of phase space onto the canonical q^i, p_i planes is preserved. This is also true of symplectic transformations in the extended phase space. Let R and R' be corresponding regions of extended phase space coordinates. Let A_i be the area of the projection of the region R onto the canonical q^i, p_i plane, and A'_i be the area of the projection of the corresponding region R' onto the canonical q'^i, p'_i plane. In the extended phase space, we also have a projection onto the t, T canonical plane. Let A_0 be the area of the projection onto the t, T plane. We have then

$$\sum_{i=0}^{n} A_i = \sum_{i=0}^{n} A'_i. \tag{5.304}$$

In terms of integrals this is

$$\sum_{i=0}^{n} \int_{R_i} dq^i dp_i = \sum_{i=0}^{n} \int_{R'_i} dq'^i dp'_i. \tag{5.305}$$

This equality for the sum of area integrals can be rewritten in terms of line integrals by Stokes' theorem:

$$\oint_{\partial R} (\sum_{i=0}^{n} p_i dq^i) = \oint_{\partial R'} (\sum_{i=0}^{n} p'_i dq'^i), \tag{5.306}$$

where the order of the integration and summation can be reversed because the boundary of R projects to the boundary on the canonical planes.

We can rephrase these results in an interesting way. Let E be the value of the Hamiltonian in the original unextended phase space. Using $q^0 = t$ and $p_0 = T = -E$ we can write

$$\sum_{i=1}^{n} \int_{R_i} dq^i dp_i - \int_{R_0} dt dE = \sum_{i=1}^{n} \int_{R'_i} dq'^i dp'_i - \int_{R'_0} dt' dE' \tag{5.307}$$

and

$$\oint_{\partial R} (\sum p_i dq^i - E dt) = \oint_{\partial R'} (\sum p'_i dq'^i - E' dt'). \tag{5.308}$$

The relations (5.307 and 5.308) are two formulations of the *Poincaré-Cartan integral invariant.*

5.7 Reduced Phase Space

Suppose we have a system with $n+1$ degrees of freedom described by a time-independent Hamiltonian in a $2n+2$ dimensional phase space. Here we can play the converse game: we can choose any generalized coordinate to play the role of "time" and the negation of its conjugate momentum to play the role of a new n degree of freedom time-dependent Hamiltonian in a *reduced phase space* of $2n$ dimensions.

More precisely, let

$$\begin{aligned} q &= \left(q^0, \ldots, q^n\right) \\ p &= [p_0, \ldots, p_n], \end{aligned} \tag{5.309}$$

and suppose we have a system described by a time-independent Hamiltonian

$$H(t, q, p) = f(q, p) = E. \tag{5.310}$$

For each solution path there is a conserved quantity E. Let's choose a coordinate q^n to be the time in a reduced phase space. We define the dynamical variables for the n degree of freedom reduced phase space:

$$\begin{aligned} q_r &= \left(q_r^0, \ldots, q_r^{n-1}\right) \\ p^r &= [p_0^r, \ldots, p_{n-1}^r]. \end{aligned} \tag{5.311}$$

In the original phase space a coordinate such as q^n maps time to a coordinate. In the formulation of the reduced phase space we will have to use the inverse function $\tau = (q^n)^{-1}$ to map the coordinate to the time, giving the new coordinates in terms of the new time

$$\begin{aligned} q_r^i &= q^i \circ \tau \\ p_i^r &= p_i \circ \tau, \end{aligned}$$

and thus

$$Dq_r^i = D(q^i \circ \tau) = (Dq^i \circ \tau)(D\tau) = (Dq^i \circ \tau)/(Dq^n \circ \tau) \tag{5.312}$$

$$Dp_i^r = D(p_i \circ \tau) = (Dp_i \circ \tau)(D\tau) = (Dp_i \circ \tau)/(Dq^n \circ \tau). \tag{5.313}$$

We propose that a Hamiltonian for our system in the reduced phase space is the negative of the inverse of $f(q^0, ..., q^n; p_0, ..., p_n) = E$ with respect to the p_n argument:

$$H_r(x, q_r, p^r) = -(\text{the } p_x \text{ such that } f(q_r, x; p^r, p_x) = E). \quad (5.314)$$

Note that in the reduced phase space we will have indices for the structured variables in the range $0 \ldots n-1$ whereas in the original phase space the indices are in the range $0 \ldots n$. We will show that H_r is an appropriate Hamiltonian for the given dynamical system in the reduced phase space. To compute Hamilton's equations we must expand the implicit definition of H_r. We define an auxiliary function

$$g(x, q_r, p^r) = f(q_r, x; p^r, -H_r(x, q_r, p^r)). \quad (5.315)$$

Note that *by construction* this function is identically a constant $g = E$. Thus all of its partial derivatives are zero:

$$\begin{aligned}\partial_0 g &= (\partial_0 f)^n - (\partial_1 f)^n \partial_0 H_r = 0\\ (\partial_1 g)_i &= (\partial_0 f)_i - (\partial_1 f)^n (\partial_1 H_r)_i = 0\\ (\partial_2 g)^i &= (\partial_1 f)^i - (\partial_1 f)^n (\partial_2 H_r)^i = 0,\end{aligned} \quad (5.316)$$

where we have suppressed the arguments. Solving for partials of H_r, we get

$$(\partial_1 H_r)_i = (\partial_0 f)_i \,/\, (\partial_1 f)^n = (\partial_1 H)_i \,/\, (\partial_2 H)^n \quad (5.317)$$

$$(\partial_2 H_r)^i = (\partial_1 f)^i \,/\, (\partial_1 f)^n = (\partial_2 H)^i \,/\, (\partial_2 H)^n\,. \quad (5.318)$$

Using these relations we can deduce the Hamilton's equations in the reduced phase space from the Hamilton's equations in the original phase space. We thus obtain Hamilton's equations in the reduced phase space:

$$\begin{aligned}Dq_r^i(x) &= \frac{Dq^i(\tau(x))}{Dq^n(\tau(x))}\\ &= \frac{(\partial_2 H(\tau(x), q(\tau(x)), p(\tau(x))))^i}{(\partial_2 H(\tau(x), q(\tau(x)), p(\tau(x))))^n}\\ &= (\partial_2 H_r(x, q_r(x), p^r(x)))^i \quad (5.319)\\ Dp_i^r(x) &= \frac{Dp_i(\tau(x))}{Dq^n(\tau(x))}\end{aligned}$$

$$= \frac{-\left(\partial_1 H(\tau(x), q(\tau(x)), p(\tau(x)))\right)_i}{\left(\partial_2 H(\tau(x), q(\tau(x)), p(\tau(x)))\right)^n}$$
$$= -(\partial_1 H_r(x, q_r(x), p^r(x)))_i. \tag{5.320}$$

Orbits in a Central Field

Consider planar motion in a central field. We have already seen this expressed in polar coordinates in equation (5.154):

$$H(t; r, \phi; p_r, p_\phi) = \frac{p_r^2}{2m} + \frac{p_\phi^2}{2mr^2} + V(r) \tag{5.321}$$

There are two degrees of freedom and the Hamiltonian is time-independent. Thus the energy, the value of the Hamiltonian, is conserved on realizable paths. Let's forget about time and reparametrize this system in terms of the orbital radius r.[23] To do this we solve

$$H(t; r, \phi; p_r, p_\phi) = E \tag{5.322}$$

for p_r, obtaining

$$H'(r; \phi; p_\phi) = -p_r = -\left(2m(E - V(r)) - \frac{p_\phi^2}{r^2}\right)^{\frac{1}{2}} \tag{5.323}$$

which is the Hamiltonian in the reduced phase space.
Hamilton's equations are now quite simple:

$$\frac{d\phi}{dr} = \frac{\partial H'}{\partial p_\phi} = \frac{p_\phi}{r^2}\left(2m(E - V(r)) - \frac{p_\phi^2}{r^2}\right)^{-\frac{1}{2}} \tag{5.324}$$
$$\frac{dp_\phi}{dr} = -\frac{\partial H'}{\partial \phi} = 0. \tag{5.325}$$

[23] We could have chosen to reparametrize in terms of ϕ, but then both p_r and r would occur in the resulting time-independent Hamiltonian. The path we have chosen takes advantage of the fact that ϕ does not appear in our Hamiltonian, so p_ϕ is a constant of the motion. This structure suggests that to solve this kind of problem we need to look ahead, as in playing chess.

We see that p_ϕ is independent of r (as it was with t), so for any particular orbit we may define a constant angular momentum L. Thus our problem ends up as a simple quadrature:

$$\phi(r) = \int^r \frac{L}{r^2}\left(2m(E - V(r)) - \frac{L^2}{r^2}\right)^{-\frac{1}{2}} dr + \phi_0. \tag{5.326}$$

To see the utility of this procedure we continue our example with a definite potential energy—a gravitating mass point:

$$V(r) = -\frac{\mu}{r} \tag{5.327}$$

When we substitute this into equation (5.326) we obtain a mess which can be simplified to

$$\phi(r) = L\int^r \frac{dr}{r\sqrt{2mEr^2 + 2m\mu r - L^2}} + \phi_0 \tag{5.328}$$

Integrating this, we obtain a further mess, which can be simplified and rearranged to obtain the following:

$$\frac{1}{r} = \frac{m\mu}{L^2}\left(1 - \sqrt{1 + \frac{2EL^2}{m\mu^2}}\sin(\phi(r) - \phi_0)\right) \tag{5.329}$$

This can be recognized as the polar-coordinate form of the equation of a conic section with eccentricity e and parameter p

$$\frac{1}{r} = \frac{1 + e\cos\theta}{p} \tag{5.330}$$

where

$$e = \sqrt{1 + \frac{2EL^2}{m\mu^2}}, \quad p = \frac{L^2}{m\mu} \quad \text{and} \quad \theta = \phi_0 - \phi(r) - \frac{\pi}{2}. \tag{5.331}$$

In fact, if the orbit is an ellipse with semimajor axis a, we have

$$p = a(1 - e^2) \tag{5.332}$$

and so we can identify the role of energy and angular momentum in shaping the ellipse:

$$E = -\frac{\mu}{2a} \quad \text{and} \quad L = \sqrt{m\mu a(1-e^2)} \tag{5.333}$$

So what we get from analysis in the reduced phase space is the geometry of the trajectory, but we lose the time-domain behavior. The reduction is often worth the price.

Although we have treated time in a special way up until now, we have found that time is not special. It can be included in the coordinates to make a driven system autonomous. And it can be eliminated from any autonomous system in favor of any other coordinate. This leads to numerous strategies for simplifying problems, by removing time variation, and then performing canonical transforms on the resulting conservative autonomous system to make a nice coordinate that we can then dump back into the role of time.

5.8 Summary

In this chapter we have investigated different representations of a dynamical system. We have found that different representations will be equivalent if the coordinate-momentum part of the transformation has symplectic derivative, and if the Hamiltonian transforms in a specified way. If the phase-space transformation is time-independent then the Hamiltonian transforms by composition with the phase-space transformation. The symplectic condition can be equivalently expressed in terms of the fundamental Poisson brackets. The Poisson-bracket and the ω function are invariant under canonical transformations. The invariance of ω implies the areas of the projections onto fundamental coordinate-momentum planes is preserved (Poincaré integral invariant) by canonical transformations.

A generating function is a real-valued function of the phase space coordinates and time that represents a canonical transformation through its partial derivatives. We found that all canonical transformations can be represented by a generating function. The proof depends on the Poincaré integral invariant (and not on the fact that total time derivatives can be added to Lagrangians without changing the equations of motion).

We can formulate an extended phase space in which time is treated as another coordinate. Time dependent transformations are simple in the extended phase space. In the extended phase space the Poincaré integral invariant is the Poincaré-Cartan integral invariant. We can also reformulate a time independent problem as a time-dependent problem with fewer degrees of freedom with one of the original coordinates taking on the role of time; this is the reduced phase space.

5.9 More Exercises

Exercise 5.9: Group Properties

a. Show that the composition of any two canonical transformations is canonical.

b. Show that composition of canonical transformations is associative.

c. Show that the identity transformation is canonical.

b. Show that there is an inverse for a canonical transformation and the inverse is canonical.

Exercise 5.10: Construction of Generating Functions

Suppose that canonical transformations C_a and C_b are generated by F_1 class generating functions F_{1a} and F_{1b}.

a. What is the generating function for the inverse transformation C_a?

b. What is the generating function for the composition transformation $C_a \circ C_b$?

Exercise 5.11: Linear Canonical Transformations

We consider systems with two degrees of freedom, and transformations for which the Hamiltonian transforms by composition.

a. Consider the linear canonical transformations that are generated by

$$F_2(x_1, x_2; p'_1, p'_2; t) = p'_1 a x_1 + p'_1 b x_2 + p'_2 c x_1 + p'_2 d x_2.$$

Show that these transformations are just the point transformations, and that the corresponding F_1 is zero.

b. Other linear canonical transformations can be generated by

$$F_1(x_1, x_2; x'_1, x'_2; t) = x'_1 a x_1 + x'_1 b x_2 + x'_2 c x_1 + x'_2 d x_2.$$

Surely we can make even more generators by constructing F_3 and F_4 class transformations analogously. Are all of the linear canonical transformations obtainable in this way? If not, show one that cannot be so generated.

c. Can all linear canonical transformations be generated by compositions of transformations generated by the functions shown in parts **a** and **b** above?

d. How many independent parameters are necessary to specify all possible linear canonical transformations for systems with two degrees of freedom?

Exercise 5.12: Integral Invariants

Consider the linear canonical transformation for a system with two degrees of freedom generated by the function:

$$F_1(x_1, x_2; x'_1, x'_2; t) = x'_1 a x_1 + x'_1 b x_2 + x'_2 c x_1 + x'_2 d x_2,$$

and the general parallelogram, with a vertex at the origin and with adjacent sides starting at the origin and extending to the phase-space points $(x_{1a}, x_{2a}, p_{1a}, p_{2a})$ and $(x_{1b}, x_{2b}, p_{1b}, p_{2b})$.

a. Find the area of the given parallelogram, and find the area of the target parallelogram under the canonical transformation. Notice that the area of the parallelogram is not preserved.

b. Find the areas of the projections of the given parallelogram, and the areas of the projections of the target under canonical transformation. Show that the sum of the areas of the projections on the action-like planes is preserved.

Exercise 5.13: Standard Map Generating Function

Find a generating function for the standard map (see exercise 5.4).

6
Continuous Transformations

Canonical transformations can be used to reformulate a problem in coordinates that are easier to understand or that expose some symmetry of a problem. In rare cases a canonical transformation can be made to a representation in which the problem is easily solvable: when all coordinate are ignorable and all the momenta are conserved. Here we investigate the Hamilton-Jacobi method for finding such canonical transformations. For problems for which the Hamilton-Jacobi method works we find that the time-evolution of the system is given as a canonical transformation.

More generally, we will find that the time evolution of any Hamiltonian system induces a canonical transformation: if we consider all possible initial states of a Hamiltonian system, and we follow all of the trajectories for the same time interval, then the map from the initial state to the final state of each trajectory is a canonical transformation. This will be true for any interval we choose, so time evolution generates a continuous family of canonical transformations.

We will generalize this idea to generate continuous canonical transformations other than that generated by time evolution. Such transformations are especially useful in analyzing dynamical systems.

6.1 Hamilton-Jacobi Equation

If we could find a canonical transformation so that the transformed Hamiltonian was identically zero, then by Hamilton's equations the new coordinates and momenta would be constants. All of the time variation of the solution would be captured in the canonical transformation, and there would be nothing more to the solution. The mixed-variable generating function that does this job satisfies a partial differential equations called the Hamilton-Jacobi equation. In most cases, the Hamilton-Jacobi equation cannot be solved explicitly. When it can be solved the Hamilton-Jacobi equation provides a means of reducing a problem to a useful simple form.

Recall the relations satisfied by an F_2 type generating function:

$$q' = \partial_2 F_2(t, q, p') \tag{6.1}$$
$$p = \partial_1 F_2(t, q, p') \tag{6.2}$$
$$H'(t, q', p') = H(t, q, p) + \partial_0 F_2(t, q, p'). \tag{6.3}$$

If we require the new Hamiltonian to be zero, then F_2 must satisfy the equation

$$0 = H(t, q, \partial_1 F_2(t, q, p')) + \partial_0 F_2(t, q, p'). \tag{6.4}$$

So the solution of the problem is "reduced" to the problem of solving an n-dimensional partial differential equation for F_2 with unspecified new (constant) momenta p'. This is the Hamilton-Jacobi equation, and in some cases we can solve it.

We can also attempt a somewhat less drastic method of solution. Rather than try to find an F_2 that makes the new Hamiltonian identically zero, we can also seek an F_2-shaped function W that gives a new Hamiltonian that is solely a function of the new momenta, for a system described by this form of Hamiltonian is also easy to solve. So if we set

$$\begin{aligned} H''(t, q'', p'') &= H(t, q, \partial_1 W(t, q, p'')) + \partial_0 W(t, q, p'') \\ &= E(p'') \end{aligned} \tag{6.5}$$

and are able to solve for W then the problem is essentially solved. In this case, the primed momenta are all constant, and the primed positions are linear in time. This is an alternate form of the Hamilton-Jacobi equation.

These forms are related. Suppose that we have a W that satisfies the second form of the Hamilton-Jacobi equation (6.5). Then the F_2 constructed from W

$$F_2(t, q, p') = W(t, q, p') - E(p')t \tag{6.6}$$

satisfies the first form of the Hamilton-Jacobi equation (6.4). Furthermore

$$p = \partial_1 F_2(t, q, p') = \partial_1 W(t, q, p'), \tag{6.7}$$

so the primed momenta are the same in the two formulations. But

$$\begin{aligned} q' &= \partial_2 F_2(t,q,p') \\ &= \partial_2 W(t,q,p') - DE(p')t \\ &= q'' - DE(p')t, \end{aligned}$$

so we see that the primed coordinates differ by a term that is linear in time—both $p'(t) = p'_0$ and $q'(t) = q'_0$ are constant. Thus we can use either W or F_2 as the generating function depending on the form of the new Hamiltonian that we want. Note that if H is time independent then from equation (6.5) we get that $\partial_0 W$ is time independent. Thus, we see that W is at most linear in time. Indeed, we can often find a time-independent W that does the job for time-independent H. In this case the Hamilton-Jacobi equation simplifies to

$$E(p') = H(t,q,\partial_1 W(t,q,p')). \tag{6.8}$$

6.1.1 Harmonic Oscillator

Consider the familiar time-independent Hamiltonian

$$H(t,x,p) = \frac{p^2}{2m} + \frac{kx^2}{2}. \tag{6.9}$$

We form the Hamilton-Jacobi equation for this problem

$$0 = H(t,x,\partial_1 F_2(t,x,p')) + \partial_0 F_2(t,q,p') \tag{6.10}$$

Using $F_2(t,x,p') = W(t,x,p') - E(p')t$ we find

$$E(p') = H(t,x,\partial_1 W(t,x,p')). \tag{6.11}$$

Writing this out explicitly

$$E(p') = \frac{(\partial_1 W(t,x,p'))^2}{2m} + \frac{kx^2}{2}, \tag{6.12}$$

and solving for $\partial_1 W$

$$\partial_1 W(t,x,p') = \sqrt{2m\left(E(p') - \frac{kx^2}{2}\right)}. \tag{6.13}$$

Integrating gives the desired W:

$$W(t,x,p') = \int^x \sqrt{2m\left(E(p') - \frac{kz^2}{2}\right)}dz. \tag{6.14}$$

We can use either W or the corresponding F_2 as the generating function. First, take W to be the generating function. We obtain the coordinate transformation by differentiating

$$\begin{aligned} x' &= \partial_2 W(t,x,p') \\ &= \int^x \frac{mDE(p')}{\sqrt{2m\left(E(p') - \frac{kz^2}{2}\right)}}dz \end{aligned} \tag{6.15}$$

and then integrating to get

$$x' = \sqrt{\frac{m}{k}}DE(p')\arcsin\left(\sqrt{\frac{k}{2E(p')}}x\right) + C(p'). \tag{6.16}$$

with some integration constant $C(p')$. Inverting this, we get the unprimed coordinate in terms of the primed coordinate and momentum

$$x = \sqrt{\frac{2E(p')}{k}}\sin\left[\frac{1}{DE(p')}\sqrt{\frac{k}{m}}(x' - C(p'))\right]. \tag{6.17}$$

The new Hamiltonian H' depends only on the momentum

$$H'(t,x',p') = E(p'). \tag{6.18}$$

The equations of motion are just

$$\begin{aligned} Dx'(t) &= \partial_2 H'(t,x'(t),p'(t)) = DE(p') \\ Dp'(t) &= -\partial_1 H'(t,x'(t),p'(t)) = 0, \end{aligned} \tag{6.19}$$

with solution

$$\begin{aligned} x'(t) &= DE(p')t + x'_0 \\ p'(t) &= p'_0 \end{aligned} \tag{6.20}$$

for initial conditions x'_0 and p'_0. If we plug these expressions for $x'(t)$ and $p'(t)$ into equation (6.17) we find

$$\begin{aligned}
x(t) &= \sqrt{\frac{2E(p')}{k}} \sin\left[\frac{1}{DE(p')}\sqrt{\frac{k}{m}}(DE(p')t + x'_0 - C(p'))\right] \\
&= \sqrt{\frac{2E(p')}{k}} \sin\left[\sqrt{\frac{k}{m}}(t - t_0)\right], \\
&= A \sin(\omega t + \phi), \qquad (6.21)
\end{aligned}$$

where the angular frequency is $\omega = \sqrt{k/m}$, the amplitude is $A = \sqrt{2E(p')/k}$, and the phase is $\phi = -\omega t_0 = \omega(x'_0 - C(p'))/DE(p')$.

We can also use $F_2 = W - Et$ as the generating function. The new Hamiltonian is zero, so both x' and p' are constant, but the relationship between the old and new variables is

$$\begin{aligned}
x' &= \partial_2 F_2(t, x, p') \\
&= \partial_2 W(t, x, p') - DE(p')t \\
&= \int^x \frac{mDE(p')}{\sqrt{2m\left(E(p') - \frac{kz^2}{2}\right)}} - DE(p')t \\
&= \sqrt{\frac{m}{k}} DE(p') \sin^{-1}\left(\sqrt{\frac{k}{2E(p')}}x\right) + C(p') - DE(p')t. \qquad (6.22)
\end{aligned}$$

Plugging in the solution $x' = x'_0$ and $p' = p'_0$ and solving for x we find equation (6.21). So once again we see that the two approaches are equivalent.

It is interesting to note that the solution depends upon the constants $E(p')$ and $DE(p')$ but otherwise the motion is not dependent in any essential way on what the function E actually is. The momentum p' is constant and the values of the constants are set by the initial conditions. Given a particular function E the initial conditions determine p', but the solution can be obtained without further specifying the E function.

If we choose particular functions E we can get particular canonical transformations. For example, a convenient choice is simply

$$E(p') = \alpha p', \qquad (6.23)$$

for some constant α that will be chosen later. We find

$$x = \sqrt{\frac{2\alpha p'}{k}} \sin \frac{\omega}{\alpha} x'. \tag{6.24}$$

So we see that a convenient choice is $\alpha = \omega = \sqrt{k/m}$, so

$$x = \sqrt{\frac{2p'}{\beta}} \sin x', \tag{6.25}$$

with $\beta = \sqrt{km}$. The new Hamiltonian is

$$H'(t, x', p') = E(p') = \omega p'. \tag{6.26}$$

The solution are just $x' = \omega t + x'_0$ and $p' = p'_0$. Substituting the expression for x in terms of x' and p' into $H(t, x, p) = H'(t, x', p')$ we derive

$$\begin{aligned} p &= \left[2m\left(p'\alpha - \frac{k}{2}x^2\right)\right]^{1/2} \\ &= \sqrt{2p'\beta} \cos x'. \end{aligned} \tag{6.27}$$

The two transformation equations (6.25) and (6.27) are what we have called the polar-canonical transformation (equation 5.34). We have already shown that this transformation is canonical and that it solves the harmonic oscillator, but it was not derived. Here we have derived this transformation as a particular case of the solution of the Hamilton-Jacobi equation.

We can also explore other choices for the E function. For example, we could choose

$$E(p') = \tfrac{1}{2}\alpha p'^2. \tag{6.28}$$

Following the same steps as before

$$x = \sqrt{\frac{\alpha p'^2}{k}} \sin \frac{\omega}{\alpha} \frac{x'}{p'}. \tag{6.29}$$

So a convenient choice is again $\alpha = \omega$ leaving

$$x = \frac{p'}{\beta} \sin \frac{x'}{p'}$$

$$p = \beta p' \cos \frac{x'}{p'}, \tag{6.30}$$

with $\beta = (km)^{1/4}$. By construction, this transformation is also canonical and also brings the harmonic oscillator problem into a easily solvable form.

$$H'(t, x', p') = \tfrac{1}{2}\omega p'^2 \tag{6.31}$$

The harmonic oscillator Hamiltonian has been transformed to what looks a lot like the Hamiltonian for a free particle. This is very interesting. Notice that whereas Hamiltonian (6.26) does not have a well defined Legendre transform to an equivalent Lagrangian, the "free particle" harmonic oscillator has a well defined Legendre transform:

$$L'(t, x', \dot{x}') = \frac{\dot{x}'^2}{2\omega}. \tag{6.32}$$

Of course, there may additional properties that make one choice more useful than others for particular applications.

Exercise 6.1: Pendulum

Solve the Hamilton-Jacobi equation for the pendulum; investigate both the circulating and oscillating regions of phase space. (Note: This requires some knowledge of elliptic functions.)

6.1.2 Kepler Problem

We can use the Hamilton-Jacobi equation to find canonical coordinates that solve the Kepler problem. This is an essential first step to doing perturbation theory for orbital problems.

In rectangular coordinates (x, y, z), the Kepler Hamiltonian is

$$H_r(t; x, y, z; p_x, p_y, p_z) = \frac{p^2}{2m} - \frac{\mu}{r}, \tag{6.33}$$

where $r^2 = x^2 + y^2 + z^2$ and $p^2 = p_x^2 + p_y^2 + p_z^2$. The Kepler problem describes the relative motion of two bodies, but it is also encountered in other problems involving orbital motion such as the n-body problem.

We try a generating function of the form $W(t; x, y, z; p'_x, p'_y, p'_z)$. The Hamilton-Jacobi equation is then[1]

$$\begin{aligned}E(p') = \frac{1}{2m}\Big[&\left(\partial_{1,0}W(t; x, y, z; p'_x, p'_y, p'_z)\right)^2 \\ &+ \left(\partial_{1,1}W(t; x, y, z; p'_x, p'_y, p'_z)\right)^2 \\ &+ \left(\partial_{1,2}W(t; x, y, z; p'_x, p'_y, p'_z)\right)^2\Big] - \frac{\mu}{r}.\end{aligned} \tag{6.34}$$

This is a partial differential equation in the three partial derivatives of W. We stare at it a while and give up.

Next we try converting to spherical coordinates. This is motivated by the appearance of r in the Hamiltonian. The Hamiltonian in spherical coordinates (r, θ, ϕ), where θ is the colatitude and ϕ is the longitude is

$$H_s(t; r, \theta, \phi; p_r, p_\theta, p_\phi) = \frac{1}{2m}\left[p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 \sin^2\theta}\right] - \frac{\mu}{r}. \tag{6.35}$$

The Hamilton-Jacobi equation is

$$\begin{aligned}&E(p'_1, p'_2, p'_3) \\ &\quad= \frac{1}{2m}\Big[\left(\partial_{1,0}W(t; r, \theta, \phi; p'_1, p'_2, p'_3)\right)^2 \\ &\qquad+ \frac{1}{r^2}\left(\partial_{1,1}W(t; r, \theta, \phi; p'_1, p'_2, p'_3)\right)^2 \\ &\qquad+ \frac{1}{r^2\sin^2\theta}\left(\partial_{1,2}W(t; r, \theta, \phi; p'_1, p'_2, p'_3)\right)^2\Big] - \frac{\mu}{r}.\end{aligned} \tag{6.36}$$

We can solve the Hamilton-Jacobi equation by successively isolating the dependence on the various variables. Looking first at the ϕ dependence, we see that, outside of W, ϕ appears only in one partial derivative. If we write

$$W(t; r, \theta, \phi; p'_1, p'_2, p'_3) = f(r, \theta, p'_1, p'_2, p'_3) + p'_3\,\phi, \tag{6.37}$$

then $\partial_{1,2}W(t; r, \theta, \phi; p'_1, p'_2, p'_3) = p'_3$, and then ϕ does not appear in the remaining equation for f:

$$E(p'_1, p'_2, p'_3)$$

[1] Remember that $\partial_{1,0}$ means the derivative with respect to the first coordinate position.

$$= \frac{1}{2m} \Big\{ (\partial_{1,0} f(r, \theta, p_1', p_2', p_3'))^2 + \frac{1}{r^2} \left[(\partial_{1,1} f(r, \theta, p_1', p_2', p_3'))^2 + \frac{(p_3')^2}{\sin^2 \theta} \right] \Big\} - \frac{\mu}{r}. \tag{6.38}$$

Any function of the p_i' could have been used as the coefficient of ϕ in the generating function. This particular choice has the nice feature that p_3' is the z component of the angular momentum.

We can eliminate the θ dependence if we choose

$$f(r, \theta, p_1', p_2', p_3') = R(r, p_1', p_2', p_3') + \Theta(\theta, p_1', p_2', p_3') \tag{6.39}$$

and require that Θ solves

$$(\partial_0 \Theta(\theta, p_1', p_2', p_3'))^2 + \frac{(p_3')^2}{\sin^2 \theta} = (p_2')^2. \tag{6.40}$$

We are free to choose the right-hand side to be any function of the new momenta; this choice reflects the fact that the left-hand side is non-negative; it turns out that p_2' is the total angular momentum. This equation for Θ can be solved by quadrature.

The remaining equation that determines R is

$$E(p_1', p_2', p_3') = \frac{1}{2m} \left[(\partial_{1,0} R(r, p_1', p_2', p_3'))^2 + \frac{1}{r^2} (p_2')^2 \right] - \frac{\mu}{r}, \tag{6.41}$$

which also can be solved by quadrature.

Altogether the solution of the Hamilton-Jacobi equation reads

$$\begin{aligned} W(r, \theta, \phi, p_1', p_2', p_3') = &\int^r \left(2mE(p_1', p_2', p_3') + \frac{2m\mu}{r} - \frac{(p_2')^2}{r^2} \right)^{1/2} dr \\ &+ \int^\theta \left((p_2')^2 - \frac{(p_3')^2}{\sin^2 \theta} \right)^{1/2} d\theta \\ &+ p_3' \phi. \end{aligned} \tag{6.42}$$

It is interesting that our solution to the Hamilton-Jacobi partial differential equation is of the form

$$\begin{aligned} &W(t; r, \theta, \phi; p_1', p_2', p_3') \\ &\quad = R(r, p_1', p_2', p_3') + \Theta(\theta, p_1', p_2', p_3') + \Phi(\phi, p_1', p_2', p_3'). \end{aligned} \tag{6.43}$$

Thus we have a separation of variables technique that involves writing the solution as a sum of functions of the individual variables. This might be contrasted with separation of variables technique encountered in elementary quantum mechanics and classical electrodynamics which use products of functions of individual variables. However, integrable problems in classical mechanics are rare, so it would be incorrect to think of this method as a general solution method.

The coordinates q'_1, q'_2, q'_3 conjugate to the momenta p'_1, p'_2, p'_3 are

$$\begin{aligned} q'_1 &= \partial_{2,0} W(t; r, \theta, \phi; p'_1, p'_2, p'_3) \\ &= m \int^r \left(2mE(p'_1, p'_2, p'_3) + \frac{2m\mu}{r} - \frac{(p'_2)^2}{r^2} \right)^{-1/2} dr \end{aligned} \tag{6.44}$$

$$\begin{aligned} q'_2 &= \partial_{2,1} W(t; r, \theta, \phi; p'_1, p'_2, p'_3) \\ &= p'_2 \int^\theta \left((p'_2)^2 - \frac{(p'_3)^2}{\sin^2\theta} \right)^{-1/2} d\theta \\ &\quad - p'_2 \int^r \frac{1}{r^2} \left(2mp'_1 + \frac{2m\mu}{r} - \frac{(p'_2)^2}{r^2} \right)^{-1/2} dr \end{aligned} \tag{6.45}$$

$$\begin{aligned} q'_3 &= \partial_{2,2} W(t; r, \theta, \phi; p'_1, p'_2, p'_3) \\ &= \phi. \end{aligned} \tag{6.46}$$

We are still free to choose the functional form of E. A convenient (and conventional) choice is

$$E(p'_1, p'_2, p'_3) = -\frac{m\mu^2}{2(p'_1)^2}. \tag{6.47}$$

With this choice the momentum p'_1 has dimensions of angular momentum, and the conjugate coordinate is an angle.

The Hamiltonian for the Kepler problem is reduced to

$$H'(t; q'_1, q'_2, q'_3; p'_1, p'_2, p'_3) = E(p'_1, p'_2, p'_3) = -\frac{m\mu^2}{2(p'_1)^2}. \tag{6.48}$$

Thus

$$q'_1 = nt + q'_{10} \tag{6.49}$$

$$q'_2 = q'_{20} \tag{6.50}$$

$$q_3' = q_{30}', \tag{6.51}$$

where $n = m\mu^2/(p_1')^3$ and where q_{10}', q_{20}', and q_{30}' are the initial values. Only one of the new variables changes with time.

The canonical phase space coordinates can be written in terms of the parameters which specify an orbit. We will just summarize the results. Assume we have a bound orbit, with semimajor axis a, eccentricity e, inclination i, longitude of ascending node Ω, argument of pericenter ω, and mean anomaly M. The three canonical momenta are

$$p_1' = \sqrt{m\mu a} \tag{6.52}$$

$$p_2' = \sqrt{m\mu a(1-e^2)} \tag{6.53}$$

$$p_3' = \sqrt{m\mu a(1-e^2)}\cos i. \tag{6.54}$$

The first momentum is related to the energy, the second momentum is the total angular momentum, and the third momentum is the component of the angular momentum in the $\hat{z}$ direction. The conjugate canonical coordinates are

$$q_1' = M \tag{6.55}$$

$$q_2' = \omega \tag{6.56}$$

$$q_3' = \Omega \tag{6.57}$$

the mean anomaly, argument of pericenter, and the longitude of the ascending node.

6.1.3 Relationship to the Action

The solution to the Hamilton-Jacobi equation, the mixed variable generating function that generates time evolution, is related to the action used in the variational principle.

Let $\widetilde{F}_2(t) = F_2(t, q(t), p'(t))$ be the value of F_2 along the paths q and p' at time t. The derivative of $\widetilde{F}_2$ is

$$\begin{aligned} D\widetilde{F}_2(t) &= \partial_1 F_2(t, q(t), p'(t)) Dq(t) \\ &\quad + \partial_2 F_2(t, q(t), p'(t)) Dp'(t) \\ &\quad + \partial_0 F_2(t, q(t), p'(t)) \\ &= p(t) Dq(t) + \partial_2 F_2(t, q(t), p'(t)) Dp'(t) \\ &\quad + \partial_0 F_2(t, q(t), p'(t)), \end{aligned} \tag{6.58}$$

where we have used the relation for p in terms of F_2 in the first term. Using the Hamilton-Jacobi equation (6.4) this becomes

$$\begin{aligned} D\widetilde{F}_2(t) &= p(t)Dq(t) - H(t, q(t), p(t)) + \partial_2 F_2(t, q(t), p'(t))Dp'(t) \\ &= L(t, q(t), Dq(t)) + \partial_2 F_2(t, q(t), p'(t))Dp'(t). \end{aligned} \tag{6.59}$$

On solution trajectories we have $Dp'(t) = 0$, so along solution trajectories the time derivative of F_2 is the same as the Lagrangian along the trajectory. The time integral of the Lagrangian along any path is the action along that path. This means that the F_2 which solves the Hamilton-Jacobi equation has the same value as the Lagrangian action for solution trajectories. Very interesting.

Harmonic Oscillator

Let's check this for the harmonic oscillator (of course).

We can finish the integral (6.14):

$$\begin{aligned} W(t, x, p') &= \int^x \sqrt{2m\left(E(p') - \frac{kz^2}{2}\right)}dz \\ &= \sqrt{mk}\tfrac{1}{2}\left[x\sqrt{A^2 - x^2} + A^2 \sin^{-1}\left(\tfrac{x}{A}\right)\right], \end{aligned} \tag{6.60}$$

with the amplitude $A = \sqrt{2E(p')/k}$.

We should check that this gives the transformation:

$$x' = \partial_2 W(t, x, p') = \sqrt{\frac{m}{k}}DE(p') \sin^{-1}\left(\frac{x}{\sqrt{2E(p')/k}}\right) \tag{6.61}$$

which is the same as equation (6.16) for a particular choice of the integration constant. The other part of the transformation is

$$p = \partial_1 W(t, x, p') = \sqrt{mk}\sqrt{A^2 - x^2}, \tag{6.62}$$

with the same definition of A as before.

Now we compute the time derivative of the associated F_2 along a solution trajectory ($Dp' = 0$):

$$\begin{aligned} D\widetilde{F}_2(t) &= \partial_1 W(t, x(t), p'_0)Dx(t) - E(p'_0) \\ &= p(t)Dx(t) - E(p'_0) \\ &= L(t, x(t), Dx(t)), \end{aligned} \tag{6.63}$$

as expected. For trajectories that are not solutions of Hamilton's equations, there are additional terms.

6.2 Time Evolution is Canonical

In this section we demonstrate that time evolution generates a canonical transformation: if we consider all possible initial states of a Hamiltonian system, and we follow all of the trajectories for the same time interval, then the map from the initial state to the final state of each trajectory is a canonical transformation.

We use time evolution to generate a transformation

$$(t, q, p) = \mathcal{C}_\Delta(t', q', p') \tag{6.64}$$

that is obtained in the following way. Let $\sigma(t) = (t, \bar{q}(t), \bar{p}(t))$ be a solution of Hamilton's equations. The transformation $\mathcal{C}_\Delta$ satisfies

$$\mathcal{C}_\Delta(\sigma(t + \Delta)) = \sigma(t), \tag{6.65}$$

or, equivalently,

$$(t, \bar{q}(t), \bar{p}(t)) = \mathcal{C}_\Delta(t + \Delta, \bar{q}(t + \Delta), \bar{p}(t + \Delta)). \tag{6.66}$$

Notice that $\mathcal{C}_\Delta$ changes the time component. This is the first transformation of this kind that we have considered.[2]

Given a state (t', q', p') we find the phase space path σ emanating from this state as an initial condition, satisfying

$$\begin{aligned} t' &= t + \Delta \\ q' &= \bar{q}(t + \Delta) \\ p' &= \bar{p}(t + \Delta). \end{aligned} \tag{6.67}$$

The value (t, q, p) of $\mathcal{C}_\Delta(t', q', p')$ is then $(t, \bar{q}(t), \bar{p}(t))$.

Time evolution is canonical if the transformation $\mathcal{C}_\Delta$ is symplectic and if the Hamiltonian transforms in an appropriate manner. The transformation $\mathcal{C}_\Delta$ is symplectic if the bilinear antisymmetric form ω is invariant (see equation 5.221) for a general pair of linearized state variations with zero time component.

---

[2]Our theorems about which transformations are still valid, because they only required that the derivative of the independent variable be 1.

Let ζ' be an increment with zero time component of the state (t', q', p'). The linearized increment in the value of $\mathcal{C}_\Delta(t', q', p')$ is $\zeta = D\mathcal{C}_\Delta(t', q', p')\zeta'$. The image of the increment is obtained by multilying the increment by the derivative of the transformation. On the other hand, the transformation is obtained by time evolution, so the image of the increment can also be found by the time evolution of the linearized variational system. Let

$$\begin{aligned}\bar\zeta(t) &= (0, \bar\zeta_q(t), \bar\zeta_p(t))\\ \bar\zeta'(t) &= (0, \bar\zeta'_q(t), \bar\zeta'_p(t))\end{aligned} \tag{6.68}$$

be variations of the state path $\sigma(t) = (t, \bar q(t), \bar p(t))$, then the requirement is

$$\begin{aligned}&\omega(\bar\zeta(t), \bar\zeta'(t))\\ &\quad = \omega(D\mathcal{C}_\Delta(\sigma(t+\Delta))\bar\zeta(t+\Delta), D\mathcal{C}_\Delta(\sigma(t+\Delta))\bar\zeta'(t+\Delta)).\end{aligned} \tag{6.69}$$

Now $D\mathcal{C}_\Delta(\sigma(t+\Delta))\bar\zeta(t+\Delta)$ is the same as $\bar\zeta(t)$. The time evolved variation is the same as the variation mapped by the time evolution transformation. So the symplectic requirement is

$$\omega(\bar\zeta(t), \bar\zeta'(t)) = \omega(\bar\zeta(t+\Delta), \bar\zeta'(t+\Delta)). \tag{6.70}$$

This condition is satisfied if

$$\begin{aligned}A(t) &= \omega(\bar\zeta(t), \bar\zeta'(t))\\ &= P(\bar\zeta'(t))Q(\bar\zeta(t) - P(\bar\zeta(t))Q(\bar\zeta'(t)\\ &= \bar\zeta'_p(t)\bar\zeta_q(t) - \bar\zeta_p(t)\bar\zeta'_q(t),\end{aligned} \tag{6.71}$$

is independent of time.

We have to compute DA:

$$\begin{aligned}DA(t) = {} & D\bar\zeta'_p(t)\bar\zeta_q(t) + \bar\zeta'_p(t)D\bar\zeta_q(t)\\ & - D\bar\zeta_p(t)\bar\zeta'_q(t) - \bar\zeta_p(t)D\bar\zeta'_q(t).\end{aligned} \tag{6.72}$$

Using Hamilton's equations the variations satisfy

$$\begin{aligned}D\bar\zeta_q(t) = {} & \partial_1\partial_2 H(t, \bar q(t), \bar p(t))\bar\zeta_q(t)\\ & + \partial_2\partial_2 H(t, \bar q(t), \bar p(t))\bar\zeta_p(t),\\ D\bar\zeta_p(t) = {} & -\partial_1\partial_1 H(t, \bar q(t), \bar p(t))\bar\zeta_q(t)\\ & - \partial_2\partial_1 H(t, \bar q(t), \bar p(t))\bar\zeta_p(t).\end{aligned} \tag{6.73}$$

Substituting these in DA and collecting terms we find[3]

$$DA(t) = 0. \tag{6.74}$$

We conclude that time evolution generates a phase space transformation with symplectic derivative.

To make a canonical transformation we must specify how the Hamiltonian transforms. The same Hamiltonian describes the evolution of a state and a time-advanced state because the latter is just another state. Thus the transformed Hamiltonian is the same as the original Hamiltonian.

Another time-evolution transformation

There is another canonical transformation that can be constructed from time evolution. We define the transformation $\mathcal{C}'_\Delta$ such that

$$\mathcal{C}'_\Delta = C_\Delta \circ S_\Delta, \tag{6.75}$$

where $S_\Delta(a, b, c) = (a+\Delta, b, c)$, is a canonical transformation that shifts the time of a phase-space state.[4] More explicitly, given a state (t, q', p'), we evolve the state that is obtained by adding Δ to t; that is, we take the state $(t + \Delta, q', p')$ as an initial state for evolution by Hamilton's equations. The state path σ satisfies

$$\begin{aligned}\sigma(t + \Delta) &= (t + \Delta, \bar{q}(t + \Delta), \bar{p}(t + \Delta))\\ &= (t + \Delta, q', p').\end{aligned} \tag{6.76}$$

The output of the transformation is the state

$$\sigma(t) = (t, \bar{q}(t), \bar{p}(t)). \tag{6.77}$$

The transformation satisfies

$$(t, \bar{q}(t), \bar{p}(t)) = \mathcal{C}'_\Delta(t, \bar{q}(t + \Delta), \bar{p}(t + \Delta)). \tag{6.78}$$

---

[3]Partial derivatives of structured arguments do not generally commute, so this deduction is not as simple as it may appear. It is helpful to introduce component indices and consider the equation componentwise.

[4]The transformation S_Δ is an identity on the qp components, so it is symplectic. Although it adjusts the time, it is not a time-dependent transformation in that the qp components do not depend upon the time. Thus, if we adjust the Hamiltonian by composition with S_Δ we will have a canonical transformation.

The arguments of $\mathcal{C}'_\Delta$ are not a consistent phase-space state, the time argument must be incremented by Δ to obtain a consistent state, and then the transformation is made by evolution of this consistent state.

Why is this a good idea? The resulting transformation is canonical, but does not change the time component. The transformation is the usual form:

$$(t, q, p) = \mathcal{C}'_\Delta(t, q', p'), \tag{6.79}$$

with the same t on both sides.

This transformation can also be extended to be a canonical transformation, with an appropriate adjustment of the Hamiltonian. The Hamiltonian H'_Δ that gives the correct Hamilton's equations at the transformed phase space point is the original Hamiltonian composed with a function that advances the independent variable by Δ:

$$H'_\Delta(t, q, p) = H(t + \Delta, q, p), \tag{6.80}$$

or

$$H'_\Delta = H \circ S_\Delta. \tag{6.81}$$

Notice that if H is time independent then $H'_\Delta = H$.

Let us assume we have a procedure `((C delta-t) state)` that implements a time-evolution transformation of the state `state` with time interval `delta-t`.

We can get a procedure `((Cp delta-t) state)` that implements $\mathcal{C}'_\Delta$ from the `((C delta-t) state)` that implements $\mathcal{C}_\Delta$ using the procedure

```
(define ((C->Cp C) delta-t)
  (compose (C delta-t) (shift-t delta-t)))
```

where `shift-t` implements S_Δ:

```
(define ((shift-t delta-t) state)
  (->H-state
   (+ (time state) delta-t)
   (coordinate state)
   (momentum state)))
```

To complete the canonical transformation we have a procedure that transforms the Hamiltonian

```
(define ((H->Hp delta-t) H)
  (compose H (shift-t delta-t)))
```

So both $\mathcal{C}$ and $\mathcal{C}'$ can be used to make canonical transformations by specifying how the old and new Hamiltonians are related. For $\mathcal{C}_\Delta$ the Hamiltonian is unchanged. For $\mathcal{C}'_\Delta$ the Hamiltonian is time-shifted .

Exercise 6.2: Verification

The condition (5.19) that Hamilton's equations are preserved for $\mathcal{C}_\Delta$ is

$$D_s H \circ \mathcal{C}_\Delta = D\mathcal{C}_\Delta \, D_s H'_\Delta,$$

and the condition (5.19) that Hamilton's equations are preserved for $\mathcal{C}'_\Delta$ is

$$D_s H \circ \mathcal{C}'_\Delta = D\mathcal{C}'_\Delta \, D_s H'_\Delta.$$

Verify that these conditions are satisfied.

Exercise 6.3: Driven Harmonic Oscillator

We can use the simple driven harmonic oscillator to illustrate that time evolution yields a symplectic transformation which can be extended to be canonical in two ways. We use the driven harmonic oscillator because its solution can be compactly expressed in explicit form.

Suppose that we have a harmonic oscillator with natural frequency ω_0 driven by a periodic sinusoidal drive of frequency ω and amplitude α. The Hamiltonian we will consider is

$$H(t, q, p) = \tfrac{1}{2}p^2 + \tfrac{1}{2}\omega_0^2 q^2 - \alpha q \cos \omega t.$$

The general solution for a given initial state (t_0, q_0, p_0) evolved for a time Δ is

$$\begin{aligned} &\begin{bmatrix} q(t_0+\Delta) \\ p(t_0+\Delta)/\omega_0 \end{bmatrix} \\ &\qquad = \begin{bmatrix} \cos\omega_0\Delta & \sin\omega_0\Delta \\ -\sin\omega_0\Delta & \cos\omega_0\Delta \end{bmatrix} \begin{bmatrix} q_0 - \alpha'\cos\omega t_0 \\ (1/\omega_0)(p_0 + \alpha'\omega\sin\omega t_0) \end{bmatrix} \\ &\qquad\quad + \begin{bmatrix} \alpha'\cos\omega(t_0+\Delta) \\ -\alpha'(\omega/\omega_0)\sin\omega(t_0+\Delta) \end{bmatrix} \end{aligned}$$

where $\alpha' = \alpha/(\omega_0^2 - \omega^2)$.

a. Fill in the details of the procedure

```
(define (((C alpha omega omega0) delta-t) state)
   ... )
```

that implements the time-evolution transformation of the driven harmonic oscillator.

b. In terms of `C` the general solution emanating from a given state is

```
(define (((solution alpha omega omega0) state0) t)
  (((C alpha omega omega0) (- (time state0) t)) state0))
```

Check that the implementation of `C` is correct by using it to construct the solution and verifying that the solution satisfies Hamilton's equations. Further check the solution by comparing to numerical integration.

c. We know that for any phase space state function F the rate of change of that function along a solution path σ is:

$$D(F \circ \sigma) = \partial_0 F \circ \sigma + \{F, H\} \circ \sigma$$

Show, by writing a short program to test it, that this is true of the function implemented by `(C delta)` for the driven oscillator. Why is this interesting?

d. Verify that both `C` and `Cp` are symplectic using the procedure `symplectic?`.

e. Use the procedure `canonical?` to verify that both `C` and `Cp` are canonical with the appropriate transformed Hamiltonian.

6.2.1 Another View of Time Evolution

We can also show that time evolution generates canonical transformations using the Poincaré-Cartan integral invariant.

Consider a two-dimensional region of phase space coordinates, R', at some particular time t' (see Figure 6.1). Let R be the image of this region at time t under time evolution for a time interval of Δ. The time evolution is governed by a Hamiltonian H. Let $\sum_i A'_i$ be the sum of the oriented areas of the projections of R' onto the fundamental canonical planes.[5] Similarly, let $\sum_i A_i$ be the sum of oriented projected areas for R. We will show that $\sum_i A_i = \sum_i A'_i$, and thus the Poincaré integral invariant is preserved by time evolution. By showing that the Poincaré integral invariant is preserved we will have shown that the qp part of the

[5]By Stoke's theorem we may compute the area of a region by a line integral around the boundary of the region. A we define the positive sense of the area to be the area enclosed by a curve that is traversed in a counterclockwise direction, when drawn on a plane with the coordinate on the abscissa and the momentum on the ordinate.

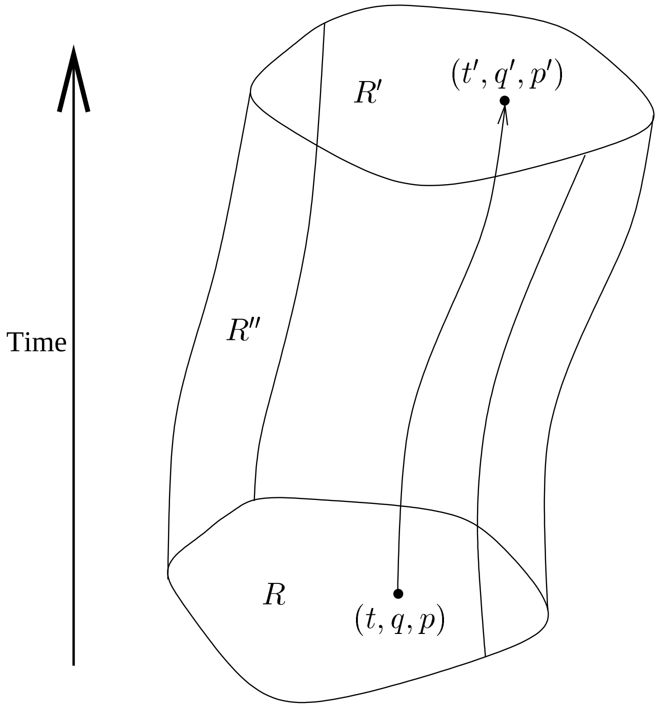

Figure 6.1 All points in some two-dimensional region R' in phase space at time t' are evolved for some time interval Δ. At the final time t the set of points define the two-dimensional region R. For example, the state labelled by the phase space coordinates (t', q', p') evolves to the state labelled by the coordinates (t, q, p).

transformation generated by time evolution is symplectic. From this we can construct canonical transformations from time evolution as before.

In the extended phase space we see that the evolution sweeps out a cylindrical volume with endcaps the regions R and R', each at a fixed time. Let R'' be the two-dimensional region swept out by the trajectories that map the boundary of region R' to the boundary of region R. The regions R, R', and R'' together form the boundary of a volume of phase state space.

The Poincaré-Cartan integral invariant on the whole boundary is zero.[6] Thus

$$-\sum_{i=0}^{n} A_i + \sum_{i=0}^{n} A_i' + \sum_{i=0}^{n} A_i'' = 0, \tag{6.82}$$

where the n index indicates the tT canonical plane. The first term is zero, because in the extended phase space we take the area to be positive if the normal to the surface is outward pointing.

We will show that the Poincaré-Cartan integral invariant for a region of phase space that is generated by time evolution is zero:

$$\sum_{i=0}^{n} A_i'' = 0. \tag{6.83}$$

This will allow us to conclude

$$-\sum_{i=0}^{n} A_i + \sum_{i=0}^{n} A_i' = 0. \tag{6.84}$$

The areas of the projection of R and R' on the tT plane are zero because R and R' are at constant times, so for these regions the Poincaré-Cartan integral invariant is the same as the Poincaré integral invariant. Thus

$$\sum_{i=1}^{n} A_i = \sum_{i=1}^{n} A_i'. \tag{6.85}$$

We are left with showing that the Poincaré-Cartan integral invariant for the region R'' is zero. This will be zero if the contribution from any small piece of R'' is zero. We will show this by showing that the ω form for a small parallelogram in this region is zero. Let $(0; q, t; p, T)$ be a vertex of this parallelogram. The parallelogram is specified by two edges ζ_1 and ζ_2 emanating from this vertex with components $(0; \Delta q, \Delta t; \Delta p, \Delta T)$. For edge ζ_1 of

[6] We can see this is the following way. Let γ be any closed curve in the boundary. This curve divides the boundary into two regions. By Stokes' theorem the integral invariant over both of these pieces can be written as a line integral along this boundary, but they have opposite signs, because γ is traversed in opposite directions to keep the surface on the left. So we conclude that integral invariant over the entire surface is zero.

the parallelogram we take a constant time phase space increment with length Δq and Δp in the q and p directions. The first order change in the Hamiltonian that corresponds to these changes is

$$\Delta H = \partial_1 H(t, q, p)\Delta q + \partial_2 H(t, q, p)\Delta p \tag{6.86}$$

for constant time $\Delta t = 0$. The increment ΔT is the negative of ΔH. So the extended phase space increment is

$$\zeta_1 = (0; \Delta q, 0; \Delta p, -\partial_1 H(t, q, p)\Delta q - \partial_2 H(t, q, p)\Delta p). \tag{6.87}$$

The edge ζ_2 is obtained by time evolution of the vertex for a time interval Δt. Using Hamilton's equations we obtain

$$\begin{aligned}\zeta_2 &= (0; Dq(t)\Delta t, \Delta t; Dp(t)\Delta t, DT(t)\Delta t)\\ &= (0; \partial_2 H(t, q, p)\Delta t, \Delta t; -\partial_1 H(t, q, p)\Delta t, -\partial_0 H(t, q, p)\Delta t).\end{aligned} \tag{6.88}$$

The ω form applied to these incremental states that form the edges of this parallelogram gives the area of the parallelogram:

$$\begin{aligned}&\omega(\zeta_1, \zeta_2)\\ &\quad = Q(\zeta_1)P(\zeta_2) - P(\zeta_1)Q(\zeta_2)\\ &\quad = (\Delta q, 0)\\ &\qquad\quad \cdot (-\partial_1 H(t, q, p)\Delta t, -\partial_0 H(t, q, p)\Delta t)\\ &\quad - (\Delta p, -\partial_1 H(t, q, p)\Delta q - \partial_2 H(t, q, p)\Delta p)\\ &\qquad\quad \cdot (\partial_2 H(t, q, p)\Delta t, \Delta t)\\ &\quad = 0.\end{aligned} \tag{6.89}$$

So we may conclude that the integral of this expression over the entire surface of the tube of trajectories is also zero. Thus the Poincaré-Cartan integral invariant is zero for any region that is generated by time evolution.

Having proven that the trajectory tube does not contribute, we have shown that the Poincaré integral invariant of the two endcaps is the same. This proves that time evolution generates a symplectic qp transformation. We have seen two ways of extending this qp transformation to canonical transformations: $\mathcal{C}_\Delta$ and $\mathcal{C}'_\Delta$. The first advances the time, and the second leaves it unchanged. For the first the Hamiltonian is unchanged, and for the second there is a time shift in the Hamiltonian.

6.2.2 Area Preservation of Surfaces of Section

We can also use the Poincaré-Cartan invariant to prove that for autonomous two degree of freedom systems surfaces of section (constructed appropriately) preserve area.

To show this we consider a surface of section for one coordinate (say q_2) equal to zero, and we construct the section by accumulating the pairs (q_1, p_1) pairs. We assume that all initial conditions have the same energy. We compute the sum of the areas of canonical projections in the extended phase space again. Because all initial conditions have the same $q_2 = 0$ there is no area on the (q_2, p_2) plane and because all the trajectories have the same value of the Hamiltonian the area of the projection on the (t, T) plane is also zero. So the sum of areas of the projections is just the area of the region on the surface of section. Now let each point on the surface of section evolve to the next section crossing. For each point on the section this may take a different amount of time. Compute the sum of the areas again for the mapped region. Again, all points of the mapped region have the same q_2 so the area on the (q_2, p_2) plane is zero, and they continue to have the same energy so the area on the (t, T) plane is zero. So the area of the mapped region is again just the area on the surface of section, the (q_1, p_1) plane. Time evolution preserves the sum of areas, so the area on the surface of section is the same as the mapped area.

So surfaces of section preserve area provided that the section points are entirely on a canonical plane. For example, for the Hénon-Heiles surfaces of section we plotted p_y versus y when $x = 0$ with $p_x \geq 0$. So for all section points the x coordinate has the fixed value 0, the trajectories all have the same energy, and the points accumulated are entirely in the (p_y, y) canonical plane. So the Hénon-Heiles surfaces of section preserve area.

6.2.3 Liouville's Theorem, Again

We have deduced that volumes in phase space are preserved by time evolution by showing that the divergence of the phase flow is zero, using the equations of motion (see section 3.8). We can also use the fact that volumes in phase space are preserved by the evolution using the fact that time evolution is a canonical transformation.

We have shown that phase space volume is preserved for symplectic transformations. Now we have shown that the transformation generated by time evolution is a symplectic transformation. Therefore, the transformation generated by time-evolution preserves phase space volume. This is an alternate proof of Liouville's theorem.

6.3 Lie Transforms

The evolution of a system under any Hamiltonian generates a continuous family of canonical transformations. We can use these transformations to help in the investigation of a system, even if its time evolution is controlled by a different Hamiltonian.

Let H be a Hamiltonian that describes the time evolution of a system under study.

Differing initial conditions give different trajectories, so really we should parameterize our trajectories by the initial state (t_0, q_0, p_0) and write

$$\sigma_{H,t_0,q_0,p_0}(t) = (t, q_{H,t_0,q_0,p_0}(t), p_{H,t_0,q_0,p_0}(t)) \tag{6.90}$$

However, these are hard to write, so we abbreviate these H-qualified trajectories with a bar: $\bar{\sigma}(t) = (t, \bar{q}(t), \bar{p}(t))$.

Let W be another Hamiltonian-shaped function defined on our phase space,[7] so it shares positions and momenta, but the state space of evolution with respect to W has a different independent variable, called τ. For each initial condition (τ_1, q_1, p_1) there is a trajectory that satisfies Hamilton's equations for W and emanates from that initial condition:

$$\sigma_{W,\tau_1,q_1,p_1}(\tau) = (\tau, q_{W,\tau_1,q_1,p_1}(\tau), p_{W,\tau_1,q_1,p_1}(\tau)) \tag{6.91}$$

Again, we abbreviate these W-qualified trajectories with a tilde: $\tilde{\sigma}(t) = (t, \tilde{q}(t), \tilde{p}(t))$.

Because Hamiltonian evolution yields symplectic transformations, we may use evolution by W to generate symplectic transformations that may be of use in studying the behavior of the system under the control of H. We define a continuous family of

---

[7]This is a new W. Do not confuse it with the mixed-variable generating function that is the solution of the second version of the Hamilton-Jacobi equation.

transformations on the phase state space of H, with parameter ϵ, $\mathcal{C}'_W(\epsilon)$ such that

$$\mathcal{C}'_W(\epsilon)(t, q', p') = (t, q_{W,\tau,q',p'}(\tau+\epsilon), p_{W,\tau,q',p'}(\tau+\epsilon)). \tag{6.92}$$

The origin of τ is arbitrary if W is independent of τ ($\partial_0 W = 0$). If W is dependent on τ then we need an additional rule to determine the origin of τ. For any ϵ this transformation has a symplectic derivative, because it is defined in terms of the evolution of a Hamiltonian system. To distinguish the Hamiltonian W that we use to generate a transformation from the Hamiltonian H that governs the time evolution of the system under study we shall call the former the *generator* of the transformation.

This transformation defines a canonical transformation if the Hamiltonian governing the time evolution of the system is transformed appropriately. If W is independent of the time parameter of H then we may extend this symplectic transformation to a canonical transformation by asserting that the Hamiltonian is transformed by composition. For a time-dependent transformation we can make a canonical transformation by adjusting the composed Hamiltonian with an additive part that makes the transformation symplectic in the extended phase space.

But if we restrict attention to time-independent generators and transformations, then we can form a canonical transformation by assuming the Hamiltonians transform by composition. So if[8]

$$(t, q, p) = \mathcal{C}'_W(\epsilon)(t, q', p'), \tag{6.93}$$

defines the transformation, and the Hamiltonian is transformed by composition

$$H' = H \circ \mathcal{C}'_W(\epsilon) \tag{6.94}$$

then the transformation is canonical.

The generator W of the canonical transformation does not need to be related to the Hamiltonian that generates the time evolution of the system under study, except that they share the same coordinates and momenta.

---

[8] We have chosen to use a $\mathcal{C}'$-type transformation because it does not advance the independent parameter. This will make it easier for us to avoid confusion with the time evolution process.

Lie Transforms of Functions

The value of a phase-space function F changes if its arguments change. We define the *Lie transform* $E'_{H,\Delta}$ of a function F of phase-space coordinates by

$$E'_{H,\Delta}F = F \circ \mathcal{C}'_{H,\Delta}. \tag{6.95}$$

Thus the Lie transform of a function satisfies

$$(E'_{H,\Delta}F)(t, q(t), p(t)) = F(t, q(t+\Delta), p(t+\Delta)) \tag{6.96}$$

for q and p solution paths of the Hamiltonian H.

In particular, the Lie transform advances the coordinate and momentum selector functions Q and P:

$$\begin{aligned}(E'_{H,\Delta}Q)(t, q(t), p(t)) &= q(t+\Delta)\\ (E'_{H,\Delta}P)(t, q(t), p(t)) &= p(t+\Delta)\end{aligned} \tag{6.97}$$

So we may restate equation (6.96) as:

$$(E'_{H,\Delta}F)(t, q, p) = F(t, ((E'_{H,\Delta}Q)(t, q, p)), ((E'_{H,\Delta}P)(t, q, p))) \tag{6.98}$$

More generally, Lie transforms descend into compositions:

$$(E'_{H,\Delta}(F \circ G)) = F \circ (E'_{H,\Delta}G) \tag{6.99}$$

Simple Lie Transforms

For example, suppose we are studying a system for which a rotation would be a helpful transformation. To concoct such a transformation we note that we intend a configuration coordinate to increase uniformly with a given rate. In this case we want an angle to be incremented. The Hamiltonian which consists solely of the momentum conjugate to that configuration coordinate always does the job. So the angular momentum is an appropriate generator for rotations.

The analysis is simple if we use polar coordinates r, θ with conjugate momenta p_r, p_θ. The generator W is just:

$$W(\tau; r, \theta; p_r, p_\theta) = p_\theta \tag{6.100}$$

The family of transformations satisfies Hamilton's equations:

$$Dr = 0$$

$$
\begin{aligned}
D\theta &= 1 \\
Dp_r &= 0 \\
Dp_\theta &= 0
\end{aligned}
\tag{6.101}
$$

Since the only variable which appears in W is p_θ then θ is the only variable that varies as ϵ is varied. In fact the family of canonical transformations is:

$$
\begin{aligned}
r &= r' \\
\theta &= \theta' + \epsilon \\
p_r &= p_r' \\
p_\theta &= p_\theta'
\end{aligned}
\tag{6.102}
$$

So angular momentum is the generator of a canonical rotation.

The example is simple, but it illustrates one important feature of Lie transformations – they give one set of variables entirely in terms of the other set of variables. This should be contrasted with the mixed-variable generating function transformations which always give a mixture of old and new variables in terms of a mixture of new and old variables, and thus require an inversion to get one set of variables in terms of the other set of variables. This inverse can only be written in closed form for special cases. In general there is considerable advantage in using a transformation rule that generates explicit transformations from the start. The Lie transformations are always explicit, in the sense that they give one set of variables in terms of the other, but for there to be explicit expressions the evolution governed by the generator must be solvable.

Let's consider another example. This time consider a three degree of freedom problem in Cartesian coordinates, and take the generator of the transformation to be the z component of the angular momentum:

$$W(\tau; x, y, z; p_x, p_y, p_z) = xp_y - yp_x \tag{6.103}$$

The evolution equations are

$$
\begin{aligned}
Dx &= -y \\
Dy &= x \\
Dz &= 0
\end{aligned}
$$

$$
\begin{aligned}
Dp_x &= -p_y \\
Dp_y &= p_x \\
Dp_z &= 0
\end{aligned}
\tag{6.104}
$$

We notice that z and p_z are unchanged; and that the equations governing the evolution of x and y decouple from those of p_x and p_y. Each of these pairs of equations represent simple harmonic motion, as can be seen by writing them as second order systems. The solutions are

$$
\begin{aligned}
x &= x' \cos\epsilon - y' \sin\epsilon \\
y &= x' \sin\epsilon + y' \cos\epsilon \\
z &= z'
\end{aligned}
\tag{6.105}
$$

$$
\begin{aligned}
p_x &= p'_x \cos\epsilon - p'_y \sin\epsilon \\
p_y &= p'_x \sin\epsilon + p'_y \cos\epsilon \\
p_z &= p'_z
\end{aligned}
\tag{6.106}
$$

So we see that again a component of the angular momentum generates a canonical rotation. There was nothing special about our choice of axes, so we can deduce that the component of angular momentum about any axis generates rotations about that axis.

Example

Suppose we have a system governed by the Hamiltonian

$$H(t; x, y; p_x, p_y) = \tfrac{1}{2}(p_x^2 + p_y^2) + \tfrac{1}{2}a(x-y)^2 + \tfrac{1}{2}b(x+y)^2. \tag{6.107}$$

Hamilton's equations couple the motion of x and y

$$
\begin{aligned}
Dx &= p_x \\
Dy &= p_y \\
Dp_x &= -a(x-y) - b(x+y) \\
Dp_y &= a(x-y) - b(x+y).
\end{aligned}
\tag{6.108}
$$

We can decouple the system by performing a coordinate rotation by $\pi/4$. This is generated by

$$W(\tau; x, y; p_x, p_y) = xp_y - yp_x, \tag{6.109}$$

which is similar to the one above but without the z degree of freedom. Evolving $(\tau; x, y; p_x, p_y)$ by W for an interval of $\pi/4$

gives a canonical rotation:

$$\begin{aligned}
x &= x' \cos \pi/4 - y' \sin \pi/4 \\
y &= x' \sin \pi/4 + y' \cos \pi/4 \\
p_x &= p'_x \cos \pi/4 - p'_y \sin \pi/4 \\
p_y &= p'_x \sin \pi/4 + p'_y \cos \pi/4.
\end{aligned} \tag{6.110}$$

Composing the Hamiltonian H with this time independent transformation gives the new Hamiltonian

$$H'(t; x', y'; p'_x, p'_y) = (\tfrac{1}{2}(p'_x)^2 + b(x')^2) + (\tfrac{1}{2}(p'_y)^2 + a(y')^2), \tag{6.111}$$

which is a Hamiltonian for two uncoupled harmonic oscillators. So the original coupled problem has been transformed by a Lie transform to a new form for which the solution is easy.

6.4 Lie Series

Taylor's theorem gives us a way of approximating the value of a nice enough function at a point near to a point where the value is known. If we know f and all of its derivatives at t then we can get the value of $f(t + \epsilon)$ for small enough ϵ, as follows:

$$f(t+\epsilon) = f(t) + \epsilon Df(t) + \frac{1}{2}\epsilon^2 D^2 f(t) + \cdots + \frac{1}{n!}\epsilon^n D^n f(t) + \cdots \tag{6.112}$$

We also recall that the power series for the exponential function is:

$$e^x = 1 + x + \frac{1}{2}x^2 + \cdots + \frac{1}{n!}x^n + \cdots \tag{6.113}$$

This suggests that we can formally construct a Taylor-series operator as the exponential of a differential operator[9]

$$e^{\epsilon D} = I + \epsilon D + \frac{1}{2}(\epsilon D)^2 + \cdots + \frac{1}{n!}(\epsilon D)^n + \cdots \tag{6.114}$$

[9] We are playing fast-and-loose with differential operators here. In a formal treatment it is essential to prove that these games are mathematically well-defined and have appropriate convergence properties.

with the goal that we will be able to write

$$f(t+\epsilon) = (e^{\epsilon D} f)(t). \tag{6.115}$$

We have to be a bit careful here: $(\epsilon D)^2 = \epsilon D \epsilon D$. We can only turn it into $\epsilon^2 D^2$ because ϵ is a scalar constant which must commute with every differential operator. But with this caveat in mind we can define the differential operator

$$(e^{\epsilon D} f)(t) = f(t) + \epsilon D f(t) + \frac{1}{2}\epsilon^2 D^2 f(t) + \cdots + \frac{1}{n!}\epsilon^n D^n f(t) + \cdots \tag{6.116}$$

Before going on, it is interesting to compute with these a bit. In the code transcripts that follow we develop the series by exponentiation. We can incrementally examine the series by looking at successive elements of the (infinite) sequence of terms of the series. The procedure `series:for-each` is an incremental traverser which applies its first argument to successive elements of the series given as its second argument. The third argument (when given) specifies the number of terms to be traversed. In each of the following transcripts we print simplified expressions for the successive terms.

The first thing to look at is the general Taylor expansion for an unknown literal function, expanded around t, with increment ϵ. Understanding what we see in this simple problem will help us understand what we will see in more complex problems later.

```
(series:for-each print-expression
 (((exp (* 'epsilon D))
   (literal-function 'f))
  't)
 6)

(f t)
(* ((D f) t) epsilon)
(* 1/2 (((expt D 2) f) t) (expt epsilon 2))
(* 1/6 (((expt D 3) f) t) (expt epsilon 3))
(* 1/24 (((expt D 4) f) t) (expt epsilon 4))
(* 1/120 (((expt D 5) f) t) (expt epsilon 5))
...
```

We can also look at the expansions of particular functions that we recognize, such as the expansion of sin around 0.

```
(series:for-each print-expression
   (((exp (* 'epsilon D)) sin) 0)
   6)

0
epsilon
0
(* -1/6 (expt epsilon 3))
0
(* 1/120 (expt epsilon 5))
...
```

It is often instructive to expand functions we usually don't remember, such as $f(x) = \sqrt{1+x}$.

```
(series:for-each print-expression
 (((exp (* 'epsilon D))
   (lambda (x) (sqrt (+ x 1))))
  0)
 6)

1
(* 1/2 epsilon)
(* -1/8 (expt epsilon 2))
(* 1/16 (expt epsilon 3))
(* -5/128 (expt epsilon 4))
(* 7/256 (expt epsilon 5))
...
```

Or, we could look at the first few terms of the binomial expansion of $(1+x)^n$:

```
(series:for-each print-expression
 (((exp (* 'epsilon D))
   (lambda (x) (expt (+ x 1) 'n)))
  0)
 6)

1
(* epsilon n)
(* (expt epsilon 2)
   (+ (* 1/2 (expt n 2))
      (* -1/2 n)))
(* (expt epsilon 3)
   (+ (* 1/6 (expt n 3))
      (* -1/2 (expt n 2))
      (* 1/3 n)))
(* (expt epsilon 4)
   (+ (* 1/24 (expt n 4))
      (* -1/4 (expt n 3))
      (* 11/24 (expt n 2))
      (* -1/4 n)))
(* (expt epsilon 5)
   (+ (* 1/120 (expt n 5))
      (* -1/12 (expt n 4))
      (* 7/24 (expt n 3))
      (* -5/12 (expt n 2))
      (* 1/5 n)))
...
```

It is amazing that for n a positive integer all of the coefficients except for the first $n+1$ are zero. (Try it for yourself! What is the value of the 5^{th} coefficient for $n = 4$? Do you now see what is going on?)

Dynamics

Now to play this game with dynamical functions we want to provide a derivative-like operator that we can exponentiate, which will give us the advance operator. The key idea is to write the derivative of the function in terms of the Poisson bracket. Equation (3.75) shows how to do this in general:

$$D(F \circ \sigma) = (\{F, H\} + \partial_0 F) \circ \sigma \tag{6.117}$$

We define the operator D_H by

$$D_H F = \partial_0 F + \{F, H\}, \tag{6.118}$$

and iterates of this operator can be used to compute higher order derivatives:

$$D^n(F \circ \sigma) = D_H^n F \circ \sigma \tag{6.119}$$

Thus we can rewrite the advance of the path function $f = F \circ \sigma$ for an interval ϵ with respect to H as a power series in the derivative operator D_H applied to the phase-space function F and then composed with the path:

$$f(t + \epsilon) = (e^{\epsilon D} f)(t) = (e^{\epsilon D_H} F) \circ \sigma(t) \tag{6.120}$$

Indeed, we can implement the time-advance operator with this series when it converges.

Exercise 6.4: Iterated Derivatives

Show that equation (6.119) is correct.

Let H be a Hamiltonian. If F and H are both time-independent, we can simplify the computation of the advance of F. In this case we define the *Lie derivative operator* L_H such that

$$L_H F = \{F, H\} \tag{6.121}$$

which reads "the Lie derivative of F with respect to H." So

$$D_H = \partial_0 + L_H \tag{6.122}$$

and for time-independent F

$$D(F \circ \sigma) = L_H F \circ \sigma \tag{6.123}$$

We can iterate this process to compute higher derivatives. So

$$L_H^2 F = \{\{F, H\}, H\}, \tag{6.124}$$

and successively higher order Poisson brackets of F with H give successively higher order derivatives when evaluated on the trajectory.

Let $f = F \circ \sigma$, we have

$$Df = (L_H F) \circ \sigma \tag{6.125}$$

$$D^2 f = (L_H^2 F) \circ \sigma \tag{6.126}$$

$$\cdots \tag{6.127}$$

Thus we can rewrite the advance of the path function f for an interval ϵ with respect to H as a power series in the Lie derivative operator applied to the phase-space function F and then composed with the path:

$$f(t+\epsilon) = (e^{\epsilon D} f)(t) = (e^{\epsilon L_H} F) \circ \sigma(t) \tag{6.128}$$

We can implement the time-advance operator $E'_{\epsilon,H}$ with the series

$$E'_{\epsilon,H} F = (e^{\epsilon L_H} F), \tag{6.129}$$

when this series converges.

We have shown that time evolution is canonical, so the series above are formal representations of canonical transformations as power series in the time. These series may not converge, even if the evolution governed by the Hamiltonian H is well defined.

Computing Lie Series

We can use the Lie transform as a computational tool to locally examine the evolution of dynamical systems. We define the Lie derivative of F, as a derivative-like operator, relative to the given Hamiltonian function, H:[10]

```
(define ((Lie-derivative H) F)
  (Poisson-bracket F H))
```

We also define a procedure to implement the Lie transform:[11]

---

[10] Actually, we define the Lie derivative slightly differently, as follows:

```
(define ((Lie-derivative-procedure H) F)
  (Poisson-bracket F H))
(define Lie-derivative
  (make-operator Lie-derivative-procedure 'Lie-derivative))
```

The reason is that we want `Lie-derivative` to be an *operator*, which is just like a function except that the product of operators is interpreted as composition while the product of functions is the function computing the product of their values.

[11] The `Lie-transform` procedure here is also defined to be an operator, just like `Lie-derivative`, but in this case the operator declaration is purely formal because the `exp` procedure will produce a series, and we do not currently have a way of iterating that process.

```
(define (Lie-transform H t)
  (exp (* t (Lie-derivative H))))
```

Let's start by examining the beginning of the Lie series for the position of a simple harmonic oscillator of mass m and spring constant k. Note that we make up the Lie transform (series) operator by passing it an appropriate Hamiltonian function and an interval to evolve for. The resulting operator is then given the `position` selector procedure. The Lie transform operator returns the new position selector procedure, that when given the phase-space coordinates `x0` and `p0` returns the position selected from the result of advancing those coordinates by the interval `dt`.

```
(series:for-each print-expression
 (((Lie-transform (H-harmonic 'm 'k) 'dt)
   state->q)
  (->H-state 0 'x0 'p0))
 6)

x0
(/ (* dt p0) m)
(/ (* -1/2 (expt dt 2) k x0) m)
(/ (* -1/6 (expt dt 3) k p0) (expt m 2))
(/ (* 1/24 (expt dt 4) (expt k 2) x0) (expt m 2))
(/ (* 1/120 (expt dt 5) (expt k 2) p0) (expt m 3))
...
```

We should recognize the terms of this series. We start with the initial position x_0. The first-order correction $(p_0/m)dt$ is due to the initial velocity. Next we find an acceleration term $(-kx_0/2m)dt^2$ due to the restoring force of the spring at the initial position.

The Lie transform is just as appropriate for showing us how the momentum evolves over the interval:

```
(series:for-each print-expression
 (((Lie-transform (H-harmonic 'm 'k) 'dt)
   state->p)
  (->H-state 0 'x0 'p0))
 6)

p0
(* -1 dt k x0)
(/ (* -1/2 (expt dt 2) k p0) m)
(/ (* 1/6 (expt dt 3) (expt k 2) x0) m)
(/ (* 1/24 (expt dt 4) (expt k 2) p0) (expt m 2))
(/ (* -1/120 (expt dt 5) (expt k 3) x0) (expt m 2))
...
```

In this series we see how the initial momentum p_0 is corrected by the effect of the restoring force $-kx_0dt$, etc.

What is a bit more fun is to see how a more complex phase-space function is treated by the Lie series expansion. In the experiment below we examine the Lie series developed by advancing the harmonic-oscillator Hamiltonian, by the transform generated by the same harmonic-oscillator Hamiltonian:

```
(series:for-each print-expression
 (((Lie-transform (H-harmonic 'm 'k) 'dt)
   (H-harmonic 'm 'k))
  (->H-state 0 'x0 'p0))
 6)

(/ (+ (* 1/2 k m (expt x0 2)) (* 1/2 (expt p0 2))) m)
0
0
0
0
0
...
```

As we would hope, the series shows us the original energy expression $(k/2)x_0^2 + (1/2m)p_0^2$ as the first term. Each subsequent correction term turns out to be zero—because the energy is conserved.

Of course, the Lie series can be used in much more complex situations where we want to see the expansion of the motion of a system characterized by a more complex Hamiltonian. The planar motion of a particle in a general central field is a simple problem for which the Lie series is instructive. In the following transcript we can see how rapidly the series becomes complicated. It is worth one's while to try to interpret the additive parts of the third (acceleration) term shown below:

```
(series:for-each print-expression
 (((Lie-transform
    (H-central-polar 'm (literal-function 'U))
    'dt)
   state->q)
  (->H-state 0
           (vector 'r_0 'phi_0)
           (vector 'p_r_0 'p_phi_0)))
 4)
(vector r_0 phi_0)
(vector (/ (* dt p_r_0) m)
        (/ (* dt p_phi_0) (* m (expt r_0 2))))
(vector
 (+ (/ (* -1/2 ((D U) r_0) (expt dt 2)) m)
    (/ (* 1/2 (expt dt 2) (expt p_phi_0 2))
       (* (expt m 2) (expt r_0 3))))
 (/ (* -1 (expt dt 2) p_phi_0 p_r_0)
    (* (expt m 2) (expt r_0 3))))
(vector
 (+ (/ (* -1/6 (((expt D 2) U) r_0) (expt dt 3) p_r_0)
       (expt m 2))
    (/ (* -1/2 (expt dt 3) (expt p_phi_0 2) p_r_0)
       (* (expt m 3) (expt r_0 4))))
 (+ (/ (* 1/3 ((D U) r_0) (expt dt 3) p_phi_0)
       (* (expt m 2) (expt r_0 3)))
    (/ (* -1/3 (expt dt 3) (expt p_phi_0 3))
       (* (expt m 3) (expt r_0 6)))
    (/ (* (expt dt 3) p_phi_0 (expt p_r_0 2))
       (* (expt m 3) (expt r_0 4)))))
...
```

Of course, if we know the closed form Lie transform it is probably a good idea to take advantage of it, but when we do not know the closed form the Lie series representation of it can come in handy.

....

6.5 Other Continuous Canonical Transformations

The Lie transform is not the only continuous canonical transformation. Another way of defining canonical transformations that depend continuously on some parameter is to introduce some parameter into a mixed variable generating function – for any value of the parameter a canonical transformation is generated. ...

6.6 Integrable Systems

A system is said to be integrable if a complete solution is known (that is, if the system can be reduced to quadratures). There is a theorem of Liouville that says that if n independent conserved quantities are known for an n degree of freedom system, then the system is reducible to quadratures. The basic idea is to make a canonical transformation to new phase space variables for which the conserved quantities are the new momenta. The new momenta are constant, so the new Hamiltonian does not depend on the coordinates conjugate to the new momenta. (*** supply proof ***)

The new momenta satisfy the fundamental Poisson bracket relations, in particular the mutual Poisson brackets of all the momenta must vanish. Poisson brackets commute with canonical transformation so a condition for this transformation to be possible is that the n conserved quantities must have vanishing mutual Poisson brackets. Phase space functions that have mutual Poisson brackets equal to zero are said to be in *involution*. For example, the three components of the angular momentum of a rigid body can be set independently by choosing appropriate initial conditions; however, the components of the angular momenta are not in involution, so they do not make suitable canonical momenta in terms of which a solution of the free rigid body may be found.

A system which can be solved by this plan is said to be *Liouville integrable*. According to Arnold [7] all known solvable problems are Liouville integrable.

7

Canonical Perturbation Theory

Closed-form solutions of dynamical systems can only rarely be found. However, even if a problem cannot be solved completely we can often obtain approximations that provide qualitative information about the dynamical system. For example, we might want to approximate the evolution; or we might want to estimate the locations and sizes of the principal regions of regular and chaotic motion.

One method of obtaining an approximate solution is by considering a system to be only slightly different from one we can solve. Suppose, for example, we have a system characterized by a Hamiltonian that breaks up into two parts as follows,

$$H = H_0 + \epsilon H_1 \tag{7.1}$$

where H_0 is solvable and ϵ is a small parameter. The difference between our system and a solvable system is then a small additive complication. The goal of perturbation theory is to investigate the full problem making use of the fact that it is close to a solvable problem.

There are many strategies for doing this. The Hamiltonian is only slightly different from the Hamiltonian of a solvable problem. We can try to find a way to transform the exact solution of this approximate problem into an approximate solution to the original problem.

We can seek a canonical transformation that eliminates the terms of order ϵ from the Hamiltonian that impede solution, leaving terms of order ϵ^2. Then seek another canonical transformation that eliminates the terms of order ϵ^2 that impede solution leaving terms of order ϵ^3. We can imagine repeating this process until the part that impedes solution is of such high order in ϵ that it can be neglected. Does this process converge? How do we know we can ever neglect the remaining terms? Let's be brave. Let's follow this path and see where it goes.

For any particular strategy we can use canonical transformations generated by mixed variable generating functions or in terms of Lie transformations. We first present a version of perturbation theory in terms of mixed variable generating functions, and then present the same strategy using Lie transformations.

7.1 Perturbation Theory with Mixed Variables

The goal is to make a canonical transformation that makes a problem look more like a nearby solvable problem. So we are interested in canonical transormations that are close to the identity transformation. Consider the transformation generated by

$$F_2(q, p', t) = p'q + \epsilon S(t, q, p'), \tag{7.2}$$

which for $\epsilon = 0$ is the identity transformation. The transformation is:

$$\begin{aligned} q' &= \partial_1 F_2(q, p', t) \\ &= q + \epsilon \partial_2 S(t, q, p') && (7.3) \\ p &= \partial_0 F_2(q, p', t) \\ &= p' + \epsilon \partial_1 S(t, q, p') && (7.4) \\ H'(t, q', p') &= H(t, q, p) + \partial_2 F_2(q, p', t) \\ &= H(t, q, p) + \epsilon \partial_0 S(t, q, p'). && (7.5) \end{aligned}$$

To complete this transformation, we need to express the unprimed variables in terms of the primed variables. In general, we may not have a closed form, but assuming that these functions are smooth enough to be expanded as series, and the difference between the primed and the unprimed variables is not too large, we may approximate

$$\begin{aligned} q &= q' - \epsilon \partial_2 S(t, q, p') \\ &= q' - \epsilon \partial_2 S(t, q' - \epsilon \partial_2 S(t, q, p'), p') \\ &= q' - \epsilon \partial_2 S(t, q', p') + \epsilon^2 (\cdots) + \cdots \end{aligned}$$

$$\begin{aligned} p &= p' + \epsilon \partial_1 S(t, q, p') \\ &= p' + \epsilon \partial_1 S(t, q' - \epsilon \partial_2 S(t, q, p'), p') \\ &= p' + \epsilon \partial_1 S(t, q', p') + \epsilon^2 (\cdots) + \cdots \end{aligned}$$

$$H'(t, q', p') = H(t, q, p) + \epsilon \partial_0 S(t, q, p')$$

$$
\begin{aligned}
&= H(t, q' - \epsilon \partial_2 S(t, q, p'), p' + \epsilon \partial_1 S(t, q, p')) \\
&\quad + \epsilon \partial_0 S(t, q' - \epsilon \partial_2 S(t, q, p'), p') \\
&= H(t, q', p') \\
&\quad + \epsilon \left[-\partial_1 H(t, q', p') \partial_2 S(t, q, p') \right. \\
&\qquad \left. + \partial_2 H(t, q', p') \partial_1 S(t, q, p') + \partial_0 S(t, q', p') \right] \\
&\quad + \epsilon^2 (\cdots) + \cdots \\
&= H(t, q', p') \\
&\quad + \epsilon \left[-\partial_1 H(t, q', p') \partial_2 S(t, q', p') \right. \\
&\qquad \left. + \partial_2 H(t, q', p') \partial_1 S(t, q', p') + \partial_0 S(t, q', p') \right] \\
&\quad + \epsilon^2 (\cdots) + \cdots
\end{aligned}
$$

Now suppose we have a Hamiltonian of the form (7.1), then

$$
\begin{aligned}
H' &= H_0 \\
&\quad + \epsilon \left(H_1 - \partial_1 H_0 \partial_2 S + \partial_2 H_0 \partial_1 S + \partial_0 S \right) \\
&\quad + \epsilon^2 (\cdots) + \cdots .
\end{aligned} \tag{7.6}
$$

The condition that there be no terms of order ϵ is

$$
H_1 - \partial_1 H_0 \partial_2 S + \partial_2 H_0 \partial_1 S + \partial_0 S = 0. \tag{7.7}
$$

Assume that H_0 depends only on the momenta: $H_0(t, q, p) = f(p)$.[1] Substituting this form for H_0 in equation (7.6) we obtain

$$
\begin{aligned}
H'(t, q', p') &= f(p') \\
&\quad + \epsilon \left(H_1(t, q', p') + Df(p') \partial_1 S(t, q', p') + \partial_0 S(t, q', p') \right) \\
&\quad + \epsilon^2 (\cdots) + \cdots
\end{aligned} \tag{7.8}
$$

So the terms of order ϵ vanish if S satisfies the partial differential equation

$$
H_1(t, q', p') + \omega_0(p') \partial_1 S(t, q', p') + \partial_0 S(t, q', p') = 0, \tag{7.9}
$$

where $\omega_0(p') = Df(p')$.

[1] The folklore is that all solvable problems can be transformed into this form. One way to carry out such a transformation is to solve the Hamilton-Jacobi equation. So we assume here that this transformation has already be performed.

If we can obtain the function S that solves equation (7.9) we can use it to carry out the required canonical transformation. The resulting Hamiltonian is of the form

$$H'(t, q', p') = f(p') + \epsilon^2(\cdots) + \cdots. \tag{7.10}$$

This Hamiltonian is of the form of equation (7.1) except that now the additional piece is of order ϵ^2 instead of order ϵ. Presumably, if we neglect the terms of order ϵ^2 we will obtain solutions that, when transformed back to the original phase space coordinates, approximate the solutions of the original problem, and these approximate solutions will be better than those obtained by neglecting the order ϵ terms in the original Hamiltonian.

Why stop here? If this process does not run into any difficulties we can iteratively remove terms of any order in ϵ and find solutions of arbitrary accuracy. Unfortunately, we do run into difficulties, and we have to modify our strategy. We can discover the difficulties by applying the method to specific problems.

Example: A pendulum

As an example of this technique we can analyze the simple pendulum as a free rotator with a perturbation due to gravity. This is a good problem to study because the actual solution is known, so by comparing the perturbation solution to the actual solution we can see how well the perturbation theory works.

The Hamiltonian for the pendulum is:

$$H(t, \theta, p_\theta) = \frac{p_\theta^2}{2\alpha} - \epsilon\beta\cos\theta, \tag{7.11}$$

where $\alpha = ml^2$ and $\beta = mgl$. The dimensionless parameter ϵ allows us to control the size of the perturbation. For this example we identify $H_0(t, \theta, p_\theta) = f(p_\theta) = p_\theta^2/(2\alpha)$ and $H_1(t, \theta, p_\theta) = -\beta\cos\theta$. We choose the mixed variable generating function

$$F_2(\theta, p'_\theta, t) = \theta p'_\theta + \epsilon S(t, \theta, p'_\theta), \tag{7.12}$$

where S satisfies

$$\omega_0(p'_\theta)\partial_1 S(t, \theta', p'_\theta) - \beta\cos\theta' + \partial_0 S(t, \theta', p'_\theta) = 0, \tag{7.13}$$

with $\omega_0(p'_\theta) = p'_\theta/\alpha$. A solution is

$$S(t, \theta', p'_\theta) = \frac{\beta \sin \theta'}{\omega_0(p'_\theta)}. \tag{7.14}$$

The Hamiltonian does not have any explicit time dependence, and neither does S. The resulting transformation is:

$$\theta = \theta' + \epsilon \frac{\alpha\beta \sin \theta'}{p'^2_\theta} + \epsilon^2(\cdots) + \cdots \tag{7.15}$$

$$p_\theta = p'_\theta + \epsilon \frac{\alpha\beta \cos \theta'}{p'_\theta} + \epsilon^2(\cdots) + \cdots, \tag{7.16}$$

and the Hamiltonian is

$$H'(t, \theta', p'_\theta) = \frac{(p'_\theta)^2}{2\alpha} + \epsilon^2(\cdots) + \cdots. \tag{7.17}$$

The first term of this Hamiltonian describes a free rotator, with a known exact solution. So if we neglect the higher order terms we can obtain an exact solution of this approximate problem. The transformation equations (7.15–7.16) allow us to find approximate solutions of the original problem in terms of the exact solutions of this approximate problem.

The plan is the following. For a given initial state (t, θ, p_θ) we use the transformation equations to find the corresponding state in the primed variables (t, θ', p'_θ). We then evolve this state in time using the Hamiltonian (7.17) with the higer order terms neglected so that the motion is solvable. We use the transformation equations again to transform this solution back to the original state variables.

Here are the details. For original initial values $\theta(0)$ and $p_\theta(0)$ we get approximate initial values in the primed coordinate system:

$$\theta'(0) = \theta(0) - \epsilon \frac{\alpha\beta \sin \theta(0)}{(p_\theta(0))^2} + \cdots \tag{7.18}$$

$$p'_\theta(0) = p_\theta(0) - \epsilon \frac{\alpha\beta \cos \theta(0)}{p_\theta(0)} + \cdots \tag{7.19}$$

The primed initial values were computed to only first order in ϵ. By re-substitution we can recursively obtain approximations that are good to any order. We can get an approximate solution in the primed system by neglecting the terms of order ϵ^2 and higher. In this approximation, the solution is

$$\begin{aligned}\theta'(t) &= \omega_0(p'_\theta(0))t + \theta'(0)\\ p'_\theta(t) &= p'_\theta(0).\end{aligned} \tag{7.20}$$

We transform these solutions back to the original state variables with the transformation equations

$$\theta(t) = \theta'(t) + \epsilon\frac{\alpha\beta\sin\theta'(t)}{(p'_\theta(t))^2} + \cdots \tag{7.21}$$

$$p_\theta(t) = p'_\theta(t) + \epsilon\frac{\alpha\beta\cos\theta'(t)}{p'_\theta(t)} + \cdots \tag{7.22}$$

That is the plan. But before seeing how well it works we note that even if it succeeds it has has only a limited range of applicability. For $|p_\theta| < (\alpha\beta\epsilon)^{1/2}$ the perturbation transformation does not represent a perturbation by a small correction (see equation 7.15). So the perturbation theory is only valid if

$$|p_\theta| > (\alpha\beta\epsilon)^{1/2}. \tag{7.23}$$

Indeed, for small $|p_\theta|$ the pendulum oscillates, and is not at all like a free rotator. In this region, it does not make sense to try to represent the solution in terms of the solution of the free rotator. However, for large p_θ, where the pendulum is rapidly circulating, the solutions of the free rotator can plausibly be deformed to approximate the solutions of the pendulum.

In the phase plane the actual solutions are just contours of the Hamiltonian. We can get an idea of how well the perturbation theory works by looking at the perturbative solutions in phase space and comparing them to the contours of the Hamiltonian (see Figure 7.1). We see that if the magnitude of the momentum is large the perturbation theory does pretty well, but for momenta near zero it is lousy.

The perturbation expressions are limited to the region for which equation (7.23) holds. It is interesting to compare this scale to the size of the oscillation region for the pendulum. We can calculate the extent of the region of oscillation of the pendulum by considering the separatrix, the trajectory that is asymptotic to the unstable equilibrium. The value of the Hamiltonian on the separatrix is the same as the value at the unstable equilibrium:

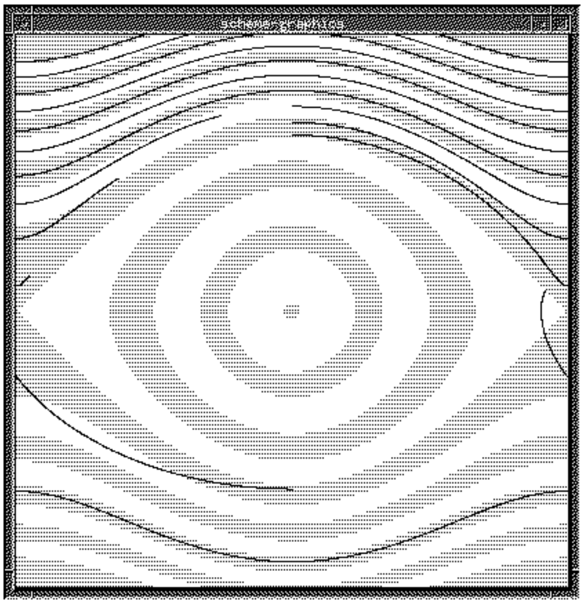

Figure 7.1 Comparison of the perturbative solution with exact motion of the pendulum. The graph shows the phase-space for our pendulum, with $\alpha = 1$ kg m^2 and $\beta = 0.1$ kg m^2/s^2. The horizontal axis shows the angle (from $-\pi$ to $+\pi$) and the vertical axis shows the angular momentum on a scale of -1 kg m^2/s to $+1$ kg m^2/s. The exact solution trajectories of the pendulum are the contours of the Hamiltonian. They have been drawn as the boundaries of the shaded regions. The dark lines are the perturbative solutions. For high energies the perturbative solution follows the contours. As the solutions approach the separatrix the perturbative solutions diverge from the actual solutions. For the outermost oscillatory solution the perturbative solution is useless, not resembling any actual solution curve.

$H(t, \theta = \pi, p_\theta = 0) = \beta\epsilon$. The separatrix has maximum momentum p_θ^{sep} at $\theta = 0$:

$$H(t, 0, p_\theta^{\text{sep}}) = H(t, \pi, 0). \tag{7.24}$$

Solving for p_θ^{sep}, the half-width of the region of oscillation, we find

$$p_\theta^{\text{sep}} = 2\sqrt{\alpha\beta\epsilon}. \tag{7.25}$$

Comparing equations (7.23) and (7.25) we see that the requirement that the terms in the perturbation solution be small excludes a region of the phase space with the same scale as the region of oscillation of the pendulum.

What the perturbation theory is doing is deforming the phase space coordinate system so that the problem looks like the free-rotor problem. This deformation is only sensible in the circulating case. So, it is not surprising that the perturbation theory fails in the oscillation region. What may be surprising is how well the perturbation theory works just outside the oscillation region. The range of p_θ in which the perturbation theory is not valid scales in the same way as the width of the oscillation region. This need not have been the case – the perturbation theory could have failed over a wider range.

7.1.1 Small Denominators

In carrying out this perturbation plan for more complicated systems we encounter additional problems. The essential step is still to solve equation (7.9), but for more complicated problems this is a partial differential equation. For many problems the coordinates are angles and if there is time dependence it is periodic. This suggests that a solution using Fourier series might be feasible.

We expand H_1 as a Fourier series[2]

$$H_1(t, q', p') = \sum_{n,m} A_{n,m}(p') \cos(nq' + m\omega t). \tag{7.26}$$

Recall that q' is a tuple of angular coordinates, and n is a tuple of integers.[3] We assume that if there is time dependence then it is periodic with frequency ω. We search for functions S that can be similarly expressed

$$S(t, q', p') = \sum_{n,m} B_{n,m}(p') \sin(nq' + m\omega t). \tag{7.27}$$

We substitute these into the determining equation (7.9) for S

$$\sum_{n,m} (n\omega_0(p') B_{n,m}(p') + A_{n,m}(p') + m\omega B_{n,m}(p')) \cos(nq' + m\omega t)$$

[2] In general we need to include sine terms in the sum, but the cosine series is often sufficient.

[3] As usual, the product of tuples is a dot product: $nq' = n_0 q'_0 + n_1 q'_1 + \cdots$.

$$= 0 \tag{7.28}$$

The components of a Fourier series are independent, so the individual coefficients must be zero:

$$B_{n,m}(p') = \frac{-1}{n\omega_0(p') + m\omega} A_{n,m}(p'). \tag{7.29}$$

If there is a term in the Fourier expansion for H_1 with both $n = 0$ and $m = 0$, then we need to modify the plan. In this case we just exclude this term from the sum for S. After the transformation, the new Hamilton is

$$H'(t, q', p') = f(p') + \epsilon A_{0,0}(p') + \epsilon^2(\cdots) + \cdots, \tag{7.30}$$

rather than Hamiltonian (7.10). The terms to first order in ϵ are still a function only of the momenta and is easily solved. The term $A_{0,0}$ is the average of H_1 over the angles and the period of the drive.

Notice that the transformation (7.27) with the coefficients (7.29) is not a perturbation if any of the denominators becomes small. So just as in the pendulum there are regions that are excluded from the domain of applicability of the perturbation theory. There is an excluded region if

$$n\omega_0(p') + m\omega \approx 0 \tag{7.31}$$

for every n and m for which there is a term $A_{n,m}$ in the Fourier expansion of H_1.

Such a failure indicates that the behavior of the physical system at or near the resonance cannot be modeled by the Fourier expansion assumed for it. As in the example of the pendulum, the problem is with the assumptions of the perturbation theory, rather than any real singularities in the motion of the system being modeled.

Example: A driven pendulum

In this example we apply our perturbation theory to the periodically driven pendulum. Recall the Hamiltonian

$$H(t, \theta, p_\theta) = \frac{p_\theta^2}{2ml^2} - ml(g + D^2 y_s(t)) \cos\theta \tag{7.32}$$

from equation (5.211), and suppose we drive it with a periodic drive, $y_s(t) = A\cos\omega t$. Then we have

$$H(t, \theta, p_\theta) = \frac{p_\theta^2}{2ml^2} - ml(g - A\omega^2\cos\omega t)\cos\theta. \tag{7.33}$$

We can expand this to see each Fourier component

$$\begin{aligned} H(t, \theta, p_\theta) = &\frac{p_\theta^2}{2ml^2} - mlg\cos\theta \\ &+ \frac{mlA\omega^2}{2}\cos(\theta + \omega t) + \frac{mlA\omega^2}{2}\cos(\theta - \omega t). \end{aligned} \tag{7.34}$$

To simplify the expressions we introduce $I = ml^2$, $\alpha = mgl$, $\gamma = mlA\omega^2/2$, so

$$H(t, \theta, p_\theta) = \frac{p_\theta^2}{2I} - \alpha\cos\theta + \beta\cos(\theta + \omega t) + \beta\cos(\theta - \omega t). \tag{7.35}$$

We can choose

$$H_0(t, \theta, p_\theta) = \frac{p_\theta^2}{2I} \tag{7.36}$$

$$H_1(t, \theta, p_\theta) = -\alpha\cos\theta + \beta\cos(\theta + \omega t) + \beta\cos(\theta - \omega t). \tag{7.37}$$

With this choice, we are thinking of the unperturbed problem as the free rotator, and the perturbation as a small gravitational field and a small drive with scale ϵ. The Fourier series for H_1 has three terms; there is no average term.

The terms of order ϵ are eliminated from the Hamiltonian if the function S satisfies the partial differential equation

$$\omega_0(p'_\theta)\partial_0 S(t, \theta', p'_\theta) + H_1(t, \theta', p'_\theta) + \partial_2 S(t, \theta', p'_\theta) = 0, \tag{7.38}$$

where

$$\omega_0(p'_\theta) = \frac{p'_\theta}{I}. \tag{7.39}$$

The series for S has three terms:

$$S(t, \theta', p'_\theta) = -\frac{\alpha\sin\theta'}{\omega_0(p'_\theta)} + \frac{\beta\sin(\theta' + \omega t)}{\omega_0(p'_\theta) + \omega} + \frac{\beta\sin(\theta' - \omega t)}{\omega_0(p'_\theta) - \omega}. \tag{7.40}$$

With this S we can produce the coordinate transformation

$$\begin{aligned}\theta \approx \theta' &+ \epsilon\frac{\alpha D\omega_0(p'_\theta)\sin\theta'}{(\omega_0(p'_\theta))^2}\\ &- \epsilon\frac{\beta D\omega_0(p'_\theta)\sin(\theta'+\omega t)}{(\omega_0(p'_\theta)+\omega)^2}\\ &- \epsilon\frac{\beta D\omega_0(p'_\theta)\sin(\theta'-\omega t)}{(\omega_0(p'_\theta)-\omega)^2}\end{aligned} \tag{7.41}$$

$$\begin{aligned}p_\theta \approx p'_\theta &- \epsilon\frac{\alpha\cos\theta'}{\omega_0(p'_\theta)}\\ &+ \epsilon\frac{\beta\cos(\theta'+\omega t)}{\omega_0(p'_\theta)+\omega}\\ &+ \epsilon\frac{\beta\cos(\theta'-\omega t)}{\omega_0(p'_\theta)-\omega}\end{aligned} \tag{7.42}$$

and the new Hamiltonian

$$H'(\theta', p'_\theta, t) = \frac{p'^2_\theta}{2I} + \epsilon^2(\cdots) + \cdots. \tag{7.43}$$

As we saw in the simple pendulum, these transformation equations become invalid when the denominators become small: if p'_θ is close to zero then $\omega_0(p'_\theta)$ is close to zero, if p'_θ is close to $I\omega$ then $\omega_0(p'_\theta) - \omega$ is close to zero, and if p'_θ is close to $-I\omega$ then $\omega_0(p'_\theta) + \omega$ is close to zero. For each denominator, an interval of p'_θ is excluded from the range of applicability of the approximation. Considering the relationship between θ and θ' we see that the range in frequency of each excluded interval is proportional to the square root of the amplitude of the corresponding perturbation term, just as it was in the case of the pendulum.

7.1.2 Nonlinear Resonances

We see that the regions excluded from the region of applicability of the perturbation theory, so far described, are the resonance regions. How can we formulate a perturbation theory that can handle the resonance regions?

The strategy just described was to eliminate as many terms in the Hamiltonian of order ϵ as possible, leaving behind lower order terms in the new variables that depend solely on the new momenta and so are solvable. However, we do not need to be so aggressive.

All we really need to do is to make sure that the new Hamiltonian is solvable.

Suppose we are interested in a particular resonance region for the driven pendulum. If we use the full generating function (7.40) then the resulting expressions will have small denominators that exclude this region from applicability. One way to eliminate this problem is to exclude from the generating function those terms that will generate the offending small denominators. It turns out that the resulting Hamiltonian is solvable.

Suppose we are interested in the region in which

$$\omega(p') - \omega \approx 0. \tag{7.44}$$

Then any term with the combination $\omega(p') - \omega$ will spoil the perturbation approximation. So we can avoid this problem by using

$$S(t, \theta', p'_\theta) = -\frac{\alpha \sin \theta'}{\omega_0(p'_\theta)} + \frac{\beta \sin(\theta' + \omega t)}{\omega_0(p'_\theta) + \omega} \tag{7.45}$$

in our generating function. The new Hamiltonian after this transformation is

$$H'(t, \theta', p') = \frac{(p')^2}{2I} + \epsilon\beta \cos(\theta - \omega t) + \epsilon^2(\cdots) + \cdots. \tag{7.46}$$

In addtion to the H_0, the term with the resonant combination of angles is left. This is not a problem, because any Hamiltonian with only a single linear combination of angles or time is solvable. We can make a canonical transformation so that this combination of angles is a new coordinate, and the resulting Hamiltonian is solvable, because all autonomous one degree-of-freedom problems are reducible to quadratures.

To reduce the leading terms of Hamiltonian (7.46) to a one degree of freedom system we make a canonical transformation to the variable $\phi = \theta - \omega t$ with the time-dependent generating function

$$F_2'(\theta', \Phi, t) = (\theta - \omega t)\Phi, \tag{7.47}$$

which implies $\phi = \theta - \omega t$, as desired, with $p' = \Phi$, and with the new resonance Hamiltonian

$$H_R(t, \phi, \Phi) = H'(t, \theta', p') - \omega\Phi$$

$$= \frac{\Phi^2}{2I} - \omega\Phi + \epsilon\beta\cos\phi \tag{7.48}$$

Neglecting an additive offset, this is

$$H_R(t, \phi, \Phi) = \frac{(\Phi - I\omega)^2}{2ml^2} + \epsilon\beta\cos\phi. \tag{7.49}$$

If we define $\Delta\Phi = \Phi - I\omega$ the Hamiltonian looks a lot like that of a pendulum

$$H_R(t, \phi, \Delta\Phi + I\omega) = \frac{(\Delta\Phi)^2}{2I} + \epsilon\beta\cos\phi. \tag{7.50}$$

The solutions follow the contours of the Hamiltonian. These are sketched in Figure (7.2).

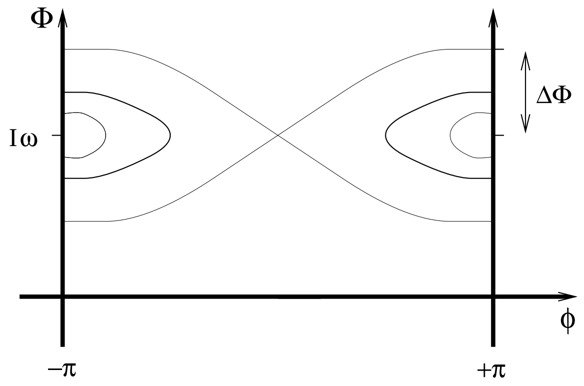

Figure 7.2 Contours of the resonance Hamiltonian are like those of the pendulum, but shifted in momentum.

7.2 Perturbation Theory with Lie Series

Carrying the mixed variable perturbation theory to higher order is very painful. The problem is that at each stage the expressions involve a mixture of old and new variables and these expressions need to be solved by recursive re-substitution for old variables in terms of new and vice versa. The result is a mess, and quickly gets out of control. A better approach to higher order perturbation theory is to use the Lie series transformations introduced earlier.

The main advantage is that the old and new variables are not ever mixed. The disadvantage of the Lie transform is that typically they are not given in closed form, but rather as an infinite series, but that is not a problem for perturbation theory because the solution is expanded as a series anyway.

We assume that the Hamiltonian has no explicit time dependence; this can be ensured by going to the extended phase space if necessary. Consider the problem

$$H(q,p) = H_0(p) + \epsilon H_1(q,p). \tag{7.51}$$

We shall perform a Lie transform with the generator $W(q,p)$ for interval ϵ to try to eliminate the order ϵ terms from the Hamiltonian.

Let's review how Lie transforms work. Taking W to be the Hamiltonian, and q and p as the initial conditions, the values of q and p an interval ϵ later will be denoted q_ϵ and p_ϵ. As a Lie series

$$q_\epsilon = \left(\mathrm{e}^{\epsilon L_W} Q\right) \circ \Pi_{q,p} \tag{7.52}$$
$$p_\epsilon = \left(\mathrm{e}^{\epsilon L_W} P\right) \circ \Pi_{q,p}, \tag{7.53}$$

where L_W denotes the Lie derivative with respect to W: $L_W x = \{x, W\}$, where the brackets indicate the Poisson bracket, and where Q and P are the coordinate and momentum selector functions. Expanding these as series we have

$$q_\epsilon = \left(Q + \epsilon\{Q,W\} + \frac{1}{2}\{\{Q,W\},W\} + \cdots\right) \circ \Pi_{q,p} \tag{7.54}$$
$$p_\epsilon = \left(P + \epsilon\{P,W\} + \frac{1}{2}\{\{P,W\},W\} + \cdots\right) \circ \Pi_{q,p}. \tag{7.55}$$

Now consider functions of the phase space, say $f(q,p)$. The function evolves solely through the evolution of the coordinates and momenta. The value of the function after evolution through the interval ϵ is

$$f_\epsilon(q,p) = \left(\mathrm{e}^{\epsilon L_W} f\right) \circ \Pi_{q,p}, \tag{7.56}$$

but since the function evolves solely through the evolution of the coordinates, we also have

$$f_\epsilon(q,p) = f(q_\epsilon, p_\epsilon) = f(\mathrm{e}^{\epsilon L_W} Q, \mathrm{e}^{\epsilon L_W} P) \circ \Pi_{q,p}, \tag{7.57}$$

So we have the fundamental theorem

$$\left(e^{\epsilon L_W} f\right) \circ \Pi_{q,p} = f(e^{\epsilon L_W} Q, e^{\epsilon L_W} P) \circ \Pi_{q,p}. \tag{7.58}$$

In applying Lie series to carry out perturbation theory we have the additional constraint that the new Hamiltonian expressed in the new variables is equal to the original Hamiltonian in the corresponding old coordinates.[4] Using the theorem about how functions transform, we find that if the coordinate and momenta transform according to equation (7.55) then the Hamiltonian governing the time evolution in the new variables is

$$H' = e^{-\epsilon L_W} H \tag{7.59}$$

so that

$$H'(q_\epsilon, p_\epsilon) = H(q, p) \tag{7.60}$$

Now let's apply this transformation to the perturbed Hamiltonian:

$$H' = e^{-\epsilon L_W} (H_0 + \epsilon H_1) \tag{7.61}$$

Writing out the first order terms in the series

$$H' = H_0 - \epsilon \{H_0, W\} + \epsilon H_1 + \epsilon^2(\cdots) + \cdots, \tag{7.62}$$

we see that to eliminate the order ϵ terms from the new Hamiltonian we must solve

$$\{H_0, W\} = H_1. \tag{7.63}$$

This is the equation that determines the generator of the Lie transformation for this stage of the perturbation theory. In detail, this equation is

$$DH_0(p)\partial_0 W(q, p) + H_1(q, p) = 0. \tag{7.64}$$

Does this look familiar? This is the same equation (7.9) that determines the mixed variable generating function S that accomplishes the same goal – the elimination of the order ϵ terms from the Hamiltonian. Though the determining equation is the

[4] Recall we are dealing with time independent Hamiltonians only.

same the consequences for higher order are completely different. The mixed variable transformation introduces a complicated sequence of higher order terms; the calculation of the higher order terms that are the consequence of the Lie series transformation is straightforward, just involving successive Poisson brackets. The expressions that relate old and new variables are unmixed from the beginning, and the inverse transformation is as easy to calculate as the original transformation.

The solution of the determining equation proceeds in the same way as in the mixed variable perturbation theory, by first writing the perturbation as a multiply periodic Fourier series and representing the generating function in the same way. Again, small denominators appear for each resonance that we attempt to remove. The Lie series provide a better organization of the perturbation theory, they do not solve the problem of the small denominators – that requires special handling of the resonances as outlined in the previous section.

7.2.1 Pendulum to Higher Order

8
Appendix: Notation

We adopt a functional mathematical notation that is close to that used by Spivak in his *Calculus on Manifolds.* The use of functional notation avoids many of the ambiguities of traditional mathematical notation; the ambiguities of traditional notation can be an impediment to clear reasoning in classical mechanics. Functional notation carefully distinguishes the function from the value of the function when applied to particular arguments. It directly supports the manipulation of functions as objects themselves.

We adopt a generic arithmetic in which the basic arithmetic operations, such as addition and multiplication, are extended to a wide variety of mathematical types. Thus, for example, the addition operator $+$ can be applied to numbers, tuples of numbers, matrices, functions, etc. The use of generic arithmetic avoids cumbersome index gymnastics.

The mathematical notation is in one-to-one correspondence with the expressions of the computer language Scheme [1]. Scheme is based on λ-calculus [5] and directly supports the manipulation of functions. We augment Scheme with symbolic, numerical, and generic features to support our applications. For a simple introduction to Scheme see appendix 9.

The correspondence between the mathematical notation and Scheme requires that mathematical expressions be unambiguous and self-contained. Scheme provides immediate feedback in verification of mathematical deductions, and facilitates the exploration of the behavior of systems.

Functions

The value of the function f given the argument x is $f(x)$. The expression $f(x)$ is not the function f.

Let f be the function that cubes its argument, $f(x) = x^3$, and let `f` be the corresponding Scheme procedure:

```
(define (f x) (* x x x))

(f 5)
125
```

Functions may be composed if the output of one is an input for the other:

$$h(x) = (f \circ g)(x) = f(g(x)).$$

Consider the procedure `h` that is the cube (`f`) of the sine (`sin`) of its input:

```
(define (h x)
  (f (sin x)))
```

The procedure `h` computes the same value as the explicit composition of `f` and `sin`, on any given input:

```
(h 2)
.7518269446689928

((compose f sin) 2)
.7518269446689928
```

Arithmetic is extended to the manipulation of functions. The usual mathematical operations may be applied to functions. Examples are addition and multiplication; we may add or multiply two functions if they take the same kinds of arguments and if their values can be added or multiplied:

$$\begin{aligned}(f+g)(x) &= f(x) + g(x) \\ (fg)(x) &= f(x)g(x).\end{aligned} \tag{8.1}$$

The Scheme arithmetic operations have been extended to accomodate this usage. Thus we may write

```
((+ f sin) 2)
8.909297426825681
```

Arithmetic is also extended to the manipulation of symbols that represent mathematical objects. By default, a Scheme symbol is assumed to represent a real number. The expression `'a` is a literal Scheme symbol.

```
(simplify ((compose f sin) 'a))
(expt (sin a) 3)
```

If instead we write

```
(define a 'b)

(simplify ((compose f sin) a))
(expt (sin b) 3)
```

we are manipulating the value of the symbol `a` rather than the symbol itself.

When dealing with symbolic expressions it is usually useful to simplify them; here we use the default simplifier to verify a trigonometric identity:

```
(simplify ((- (+ (square sin) (square cos)) 1) 'a))
0
```

Just as it is useful to be able to manipulate symbolic numbers, it is useful to be able to manipulate symbolic functions. The procedure `literal-function` makes a procedure that acts as a function having no properties other than its name:

```
(simplify ((literal-function 'g) 'x))
(g x)

(simplify ((+ (compose square (literal-function 'g)) sin) 'x))
(+ (expt (g x) 2) (sin x))
```

Derivatives

The derivative of a function f is a function. It is denoted by Df. Our notational convention is that D is a high-precedence operator. Thus D operates on the adjacent function before any other application occurs: $Df(x)$ is the same as $(Df)(x)$.

The derivative of a function f is the function Df whose value for a particular argument is something that can be multiplied by an increment in the argument Δx to get a linear approximation to the increment in the value of f:

$$f(x + \Delta x) \approx f(x) + Df(x)\Delta x. \tag{8.2}$$

For example, let f be the function that cubes its argument ($f(x) = x^3$), then Df is the function that yields three times the square of its argument ($Df(y) = 3y^2$). We may apply a function at a particular argument, so $f(5) = 125$ and $Df(5) = 75$.

For our example above,

$$f(x + \Delta x) = (x + \Delta x)^3 = x^3 + 3x^2\Delta x + 3x\Delta x^2 + \Delta x^3 \tag{8.3}$$

and

$$Df(x)\Delta x = 3x^2\Delta x. \tag{8.4}$$

So $Df(x)$ multiplied by Δx gives us the term in $f(x + \Delta x)$ that is linear in Δx, providing a good approximation to the increment in the function $f(x + \Delta x) - f(x)$ when Δx is a small increment.

The Scheme procedure for producing the derivative of a function is named `D`.

```
((D f) 5)
75
```

If we supply symbolic arguments we obtain symbolic results:

```
(simplify ((D (compose square sin)) 'a))
(* 2 (sin a) (cos a))
```

Higher-order derivatives are described by exponentiating the derivative operator. Thus the nth derivative of a function f is notated by $D^n f$. We can do this in Scheme as well:

```
(simplify (((expt D 2) (compose square sin)) 'a))
(+ -2 (* 4 (expt (cos a) 2)))
```

Notice that if `D` were an ordinary function, then the rule for multiplication would imply that `((expt D 2) f)` would just be the product of the derivative of the function `f` with itself. But derivatives are operators. An operator is like a function except that multiplication of operators is composition, whereas multiplication of functions is multiplication of the values (see equation 8.1) Arithmetic is extended to allow manipulation of operators. A typical operator is

$$(D + 1)(D - 1) = D^2 - 1.$$

Such an operator can be constructed and used in Scheme:

```
(simplify (((* (- D 1) (+ D 1)) (literal-function 'f)) 'x))
(+ (((expt D 2) f) x) (* -1 (f x)))
```

In this context a number is treated as an operator that multiplies its input by the number.

Tuples

It is often useful to manipulate an aggregate of quantities as a single unit. Such an aggregate is called a tuple. For example, the polar coordinates r, θ, φ of a point can be aggregated to form the tuple $q = (r, \theta, \varphi)$. We use zero-based indexing when referring to tuple elements.

Tuple arithmetic is inspired by tensor arithmetic, but it is more general: not all of the components of a tuple need to be of the same size or type.

We distinguish two types of tuples, which we call "up tuples" and "down tuples." A component of an up tuple is usually identified with a superscript. A component of a down tuple is identified with a subscript. For example, a three-dimensional vector can be written as a linear combination of basis elements $\hat{e}_0$, $\hat{e}_1$, and $\hat{e}_2$:

$$\vec{v} = v^0 \hat{e}_0 + v^1 \hat{e}_1 + v^2 \hat{e}_2. \tag{8.5}$$

The coefficients of the combination are the components v^0, v^1, and v^2 of a coordinate tuple v:

$$v = \left(v^0, v^1, v^2\right). \tag{8.6}$$

We write tuples as ordered lists of their components; a tuple is delimited by parentheses if it is an up tuple and it it delimited by square brackets if it is a down tuple. For example, the down tuple p of momentum components p_0, p_1, and p_2 is

$$p = [p_0, p_1, p_2]. \tag{8.7}$$

Two up tuples may be added or subtracted, elementwise, to produce an up tuple. Similarly, two down tuples may be added or subtracted, elementwise, to produce a down tuple.

Two tuples are said to be compatible for multiplication if they are of opposite types, they are of the same length, and their corresponding elements are compatible for multiplication. Any tuple may be multiplied by a number, by multiplying each component by the number. Numbers may, of course, be multiplied.

An up tuple of numbers can be multiplied by a down tuple of numbers if they have the same number of elements. The result is the sum of the products of corresponding components of the tuples. Multiplication of compatible tuples is commutative. So the product of p and v is

$$pv = vp = p_0 v^0 + p_1 v^1 + p_2 v^2. \tag{8.8}$$

In Scheme we make tuples with the constructors `up` and `down`. For mnemonic value we make specific constructors for particular kinds of tuples. So the constructors `coordinate-tuple`, `velocity-tuple`, and `acceleration-tuple` make up tuples and the constructor `momentum-tuple` makes a down tuple.

```
(simplify (velocity-tuple 4 3 2))
(up 4 3 2)
(simplify (momentum-tuple 1 2 3))
(down 1 2 3)
(* (momentum-tuple 1 2 3) (velocity-tuple 4 3 2))
16
```

Tuples may contain other tuples as components. As a consequence of this, multiplication of compatible tuples is not associative.

```
(* (* (up 5 2) (down (down 3 5) (down 7 9))) (up 11 13))
878

(* (up 5 2) (* (down (down 3 5) (down 7 9)) (up 11 13)))
964
```

Tuple structures can be made to represent linear transformations. For example, the rotation commonly represented by the matrix

$$\begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \tag{8.9}$$

can be represented as a tuple structure,

$$\left[\begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix} \right] \tag{8.10}$$

which can be made by the program:

```
(down (up (cos theta) (sin theta))
      (up (- (sin theta)) (cos theta)))
```

Such a tuple is compatible for multiplication with an up tuple that represents a vector. So, for example:

$$\left[\begin{pmatrix}\cos\theta\\ \sin\theta\end{pmatrix}\begin{pmatrix}-\sin\theta\\ \cos\theta\end{pmatrix}\right]\begin{pmatrix}x\\ y\end{pmatrix}=\begin{pmatrix}x\cos\theta-y\sin\theta\\ x\sin\theta+y\cos\theta\end{pmatrix} \tag{8.11}$$

Two tuple structures that represent linear transformations are are not compatible for multiplication but we want to use multiplication to compose such transformations, so we extend the multiplication to handle this case. The multiplication of tuple structures that represent linear transformations is associative but not commutative.

Derivatives of Functions of Multiple Arguments

The derivative generalizes to functions that take multiple arguments. If a function maps several real arguments to a real value, then if we take a step in the argument space described by an incremental vector, we must be able to multiply the derivative of the function by the incremental vector to get a linear approximation to the resulting increment of the function value. The derivative of a real-valued function of multiple arguments is an object whose inner product with the incremental vector gives the function increment. If the incremental vector is represented as an up tuple of components, one for each argument position, then the derivative can be represented as a down tuple of the partial derivatives of the function with respect to each argument.

Suppose we have a real-valued function g of two real-valued arguments, and we want to approximate the increment in the value of g from its value at x, y. If the arguments are incremented by the tuple $\Delta v = (\Delta x, \Delta y)$ we compute:

$$\begin{aligned} Dg(x,y)\Delta v &= [\partial_0 g(x,y), \partial_1 g(x,y)] \cdot (\Delta x, \Delta y) \\ &= \partial_0 g(x,y)\Delta x + \partial_1 g(x,y)\Delta y. \end{aligned} \tag{8.12}$$

In general, partial derivatives are just the components of the derivative of a function that takes multiple arguments (or structured arguments or both, see below). So a partial derivative of a function is a composition of a component selector and the derivative of that function. Indeed:

$$\partial_0 g = (Dg)_0 \tag{8.13}$$

$$\partial_1 g = (Dg)_1. \tag{8.14}$$

Concretely, if

$$g(x, y) = x^3 y^5 \tag{8.15}$$

then

$$Dg(x, y) = \left[3x^2y^5, 5x^3y^4\right] \tag{8.16}$$

and the first-order approximation of the increment for changing the arguments by $\Delta x, \Delta y$ is

$$\begin{aligned} g(x + \Delta x, y + \Delta y) - g(x, y) &\approx \left[3x^2y^5, 5x^3y^4\right] \cdot (\Delta x, \Delta y) \\ &= 3x^2y^5\Delta x + 5x^3y^4\Delta y. \end{aligned} \tag{8.17}$$

As a computer program, we may write

```
(define (g x y)
  (* (expt x 3) (expt y 5)))

(simplify ((D g) 'a 'b))
(down (* 3 (expt a 2) (expt b 5))
      (* 5 (expt a 3) (expt b 4)))
```

and the inner product with an incremental vector is the appropriate increment.

```
(simplify (* ((D g) 'a 'b) (up 'da 'db)))
(+ (* 3 da (expt a 2) (expt b 5))
   (* 5 db (expt a 3) (expt b 4)))
```

Structured Arguments

We like to think of a function of a single tuple as a function of its components:

$$h(v) = h(v^0, v^1, \ldots). \tag{8.18}$$

Scheme is too strict to allow this. In Scheme we distinguish a single tuple argument from multiple arguments. For example, a procedure that computes the same value as g (see equation 8.15) is written

```
(define (h v)
  (let ((x (ref v 0)) (y (ref v 1)))
    (* (expt x 3) (expt y 5))))

(simplify (h (up 'a 'b)))
(* (expt a 3) (expt b 5))
```

However, the derivative of `g` and `h` must have the same value for equivalent inputs: the value of the derivative when multiplied by an increment in the input produces an increment in the function. The increments to the arguments of `g` and `h` are both specified as up tuples of incremental components, so the derivatives must have the same shape:

```
(simplify ((D h) (up 'a 'b)))
(down (* 3 (expt a 2) (expt b 5))
      (* 5 (expt a 3) (expt b 4)))
```

which is the same as `((D g) 'a 'b)` computed above.

Things get somewhat more complicated when we have functions with multiple structured arguments. Consider a function whose first argument is an up tuple and whose second argument is a number:

```
(define (k v w)
  (+ (h v) (cube w)))
```

Now what is its derivative? Well, it had better be something that can multiply an increment in the arguments to get an increment in the function. The increment in the first argument is an incremental up tuple. The increment in the second argument is a small number. Thus we need a down tuple of two parts, a down-tuple of the values of the partial derivatives with respect to each component of the first argument and the value of the partial derivative with respect to the second argument. This is easier to see symbolically:

```
(simplify ((derivative k) (up 'a 'b) 'c))
(down (down (* 3 (expt a 2) (expt b 5))
            (* 5 (expt a 3) (expt b 4)))
      (* 3 (expt c 2)))
```

The idea generalizes.

As before, partial derivatives are just the components of the derivative of a function that takes multiple arguments or structured arguments or both. Thus, a partial derivative of a function is a composition of a component selector and the derivative of that function. The procedure that makes a partial derivative operator given a selection chain is named `partial`.

```
(simplify (((partial 0) k) (up 'a 'b) 'c))
(down (* 3 (expt a 2) (expt b 5))
      (* 5 (expt a 3) (expt b 4)))

(simplify (((partial 1) k) (up 'a 'b) 'c))
(* 3 (expt c 2))

(simplify (((partial 0 0) k) (up 'a 'b) 'c))
(* 3 (expt a 2) (expt b 5))

(simplify (((partial 0 1) k) (up 'a 'b) 'c))
(* 5 (expt a 3) (expt b 4))
```

This naming scheme is consistent, except for one special case. If a function takes exactly one structured argument then one level of the structure hierarchy is eliminated, allowing one to naturally write:

```
(simplify ((D h) (up 'a 'b)))
(down (* 3 (expt a 2) (expt b 5))
      (* 5 (expt a 3) (expt b 4)))

(simplify (((partial 0) h) (up 'a 'b)))
(* 3 (expt a 2) (expt b 5))

(simplify (((partial 1) h) (up 'a 'b)))
(* 5 (expt a 3) (expt b 4))
```

Besides arguments that are up tuples of components, we also have arguments that are down tuples of components. Since the derivative of h produces a down tuple as its value, any function, say s, that can be composed with h must take a down tuple as its argument. The derivative of s must be something that can be multiplied by an incremental down tuple to produce an approximation to the increment in the value of s: it must produce an up tuple of partial derivatives. Thus we have the rule that the derivative of a function that takes an up tuple is a down tuple and the derivative of a function that takes a down tuple is an up tuple.

This can get quite elaborate when we have a function of multiple structured arguments of mixed type, where some arguments are up tuples and others are down tuples. For example, consider a procedure that takes an up tuple of three components: the first is a number, the second is an up tuple, and the third is a down tuple. The derivative of this function must be a function that produces an object that can be multiplied by an increment in the argument structure to produce an increment in the function's value. Thus we see that the derivative must be a down tuple of three partial derivatives. The first partial derivative is the partial derivative wtih respect to the numerical argument. The second partial derivative is a down tuple of partial derivatives, with respect to each component of the up-tuple argument. The third partial derivative is an up tuple of partial derivatives, with repect to each component of the down-tuple argument.

Please be warned: partial derivative operators with respect to different structured arguments do not commute.

Structured Results

Some functions produce multiple outputs. For example, a function that takes one numerical argument and produces a structure of outputs may be used to describe a curve through space. The following function describes a linearly expanding helical path around the z-axis in three-dimensional space:

```
(define (helix t)
  (up (* t (cos t)) (* t (sin t)) t))
```

Its derivative is just the up tuple of the derivatives of each component of the function:

```
(simplify ((D helix) 't))
(up (+ (* -1 t (sin t)) (cos t))
    (+ (* t (cos t)) (sin t))
    1)
```

These components specify the velocities at time t in each coordinate direction.

In general, a function that produces multiple outputs is just treated as a structure of functions, one for each of the outputs. The derivative of a function of multiple inputs that produces multiple outputs is an object that when multiplied by an incremental input produces a linear approximation to the incremental output. Thus:

```
(define (g1 x y)
  (up (square (+ x y)) (cube (- y x)) (exp (+ x y))))

(print-expression ((D g1) 'x 'y))
(down (up (+ (* 2 x) (* 2 y))
  (+ (* -3 (expt x 2)) (* 6 x y) (* -3 (expt y 2)))
  (* (exp y) (exp x)))
      (up (+ (* 2 x) (* 2 y))
  (+ (* 3 (expt x 2)) (* -6 x y) (* 3 (expt y 2)))
  (* (exp y) (exp x))))
```

Exercise 8.1: Chain Rule

Let $F(x, y) = x^2y^3$, $G(x, y) = (F(x, y), y)$, and $H(x, y) = F(F(x, y), y)$, so that $H = F \circ G$.

a. Compute $\partial_0 F(x, y)$, and $\partial_1 F(x, y)$.

b. Compute $\partial_0 F(F(x, y), y)$, and $\partial_1 F(F(x, y), y)$.

c. Compute $\partial_0 G(x, y)$, and $\partial_1 G(x, y)$.

d. Compute $DF(a, b)$, $DG(3, 5)$, and $DH(3a^2, 5b^3)$.

Exercise 8.2: Computing Derivatives

We can represent functions of multiple arguments as procedures in several ways, depending upon how we wish to use them. The simplest idea is to identify the procedure arguments with the function's arguments.

For example, we could write implementations of the functions that occur in Exercise 8.1 as follows:

```
(define (f x y)
  (* (square x) (cube y)))

(define (g x y)
  (up (f x y) y))

(define (h x y)
  (f (f x y) y))
```

With this choice it is awkward to compose a function with multiple arguments with a function that produces a tuple of those arguments. Alternatively, we can represent the function arguments as slots of a vector data structure, and then composition with a function that produces such a data structure is easy. However, this choice requires the procedures to build and take apart structures.

For example, we may define procedures that implement the functions above as follows:

```
(define (f v)
  (let ((x (ref v 0))
        (y (ref v 1)))
    (* (square x) (cube y))))

(define (g v)
  (let ((x (ref v 0))
        (y (ref v 1)))
    (up (f v) y)))

(define h (compose f g))
```

Repeat Exercise 8.1 using the computer. Explore both implementations of multiple argument functions.

9

Appendix: Scheme

Here we give an elementary introduction to Scheme.[1] For a more precise explanation of the language see the IEEE standard [1]. For a longer introduction see the textbook [2].

Scheme is a simple programming language based on expressions. An expression names a value. For example, the numeral `3.14` names an approximation to a familiar number. There are primitive expressions, such as a numeral, that we directly recognize, and there are compound expressions of several kinds.

A procedure call is a kind of compound expression. A procedure call is a sequence of expressions delimited by parentheses. The first subexpression in a procedure call is taken to name a procedure, and the rest of the subexpressions are taken to name the arguments to that procedure. The value of the procedure when applied to the given arguments is the value named by the procedure call. For example,

```
(+ 1 2.14)
3.14

(+ 1 (* 2 1.07))
3.14
```

are both compound expressions that name the same number as the numeral 3.14.[2] In these cases the symbols `+` and `*` name procedures that add and multiply, respectively. If we replace any subexpression of any expression with an expression that names the same thing as the original subexpression named, the thing named by the overall expression remains unchanged. In general, a procedure call is

(*operator* *operand-1* ... *operand-n*)

---

[1]Many of the statements here are only valid assuming there are no assignments.

[2]In examples we show the value that would be printed by the Scheme system using an italic face following the input expression.

where *operator* names a procedure and *operand-i* names the ith argument.[3]

Just as we use numerals to name numbers, we can use λ-expressions to name procedures. For example, the procedure that squares its input can be written:

```
(lambda (x) (* x x))
```

This expression can be read: "The procedure of one argument, x, that multiplies x by x." Of course, we can use this expression in any context where a procedure is needed. For example,

```
((lambda (x) (* x x)) 4)
16
```

The general form of a λ-expression is:

(lambda *formal-parameters body*)

where *formal-parameters* is a list of symbols that will be the names of the arguments to the procedure and the body is an expression that may refer to the formal parameters. The value of a procedure call is the value of the body of the procedure with the arguments substituted for the formal parameters.

We can use the `define` construct to give a name to any object. For example, if we make the definitions

```
(define pi 3.141592653589793)

(define square (lambda (x) (* x x)))
```

we can then use the symbols `pi` and `square` wherever the numeral or the λ-expression could appear. For example, the area of the surface of a sphere of radius 4 meters is:

```
(* 4 pi (square 4))
201.06192982974676
```

Procedure definitions may be expressed more conveniently, using syntactic sugar. The squaring procedure may be defined

```
(define (square x) (* x x))
```

---

[3] In Scheme every parentheses is essential: you cannot add extra parentheses or remove any.

which we may read: "To square x multiply x by x."

In Scheme, procedures may be passed as arguments and returned as values. For example, it is possible to make a procedure that implements the mathematical notion of the composition of two functions:[4]

```
(define compose
  (lambda (f g)
    (lambda (x)
      (f (g x)))))

((compose square sin) 2)
.826821810431806

(square (sin 2))
.826821810431806
```

Using the same syntactic sugar we can write the definition more conveniently. The following are both equivalent to the definition above:

```
(define (compose f g)
  (lambda (x)
    (f (g x))))

(define ((compose f g) x)
  (f (g x)))
```

Conditional expressions may be used to choose among several expressions to produce a value. For example, a procedure that implements the absolute value function may be written:

```
(define (abs x)
  (cond ((< x 0) (- x))
        ((= x 0) x)
        ((> x 0) x)))
```

The conditional `cond` takes a number of clauses. Each clause has a predicate expression, which may be either true or false, and a consequent expression. The value of the `cond` expression is the value of the consequent expression of the first clause for which the

[4]The examples are indented to help with readability. Scheme does not care about extra whitespace, so we may add as much as we please to make things easier to read.

predicate expression is true. The general form of a conditional expression is

```
(cond ( predicate-1  consequent-1)
      ...
      ( predicate-n  consequent-n))
```

For convenience there is a special predicate expression `else` that can be used as the predicate in the last clause of a `cond`. The `if` construct provides another way to make a conditional when there is only a binary choice to be made. For example, because we only have to do something special when the argument is negative we could have defined `abs` as:

```
(define (abs x)
  (if (< x 0)
      (- x)
      x))
```

The general form of an `if` expression is

```
(if  predicate  consequent  alternative)
```

If the *predicate* is true the value of the `if` expression is the value of the *consequent*, otherwise it is the value of the *alternative*.

Given conditionals and definitions we can write recursive procedures. For example, to compute the nth factorial number we may write:

```
(define (factorial n)
  (if (= n 0)
      1
      (* n (factorial (- n 1)))))

(factorial 6)
720

(factorial 40)
815915283247897734345611269596115894272000000000
```

The `let` expression is used to give names to objects in a local context. For example,

```
(define (f r)
  (let ((area (* 4 pi (square r)))
        (volume (* 4/3 pi (cube r))))
    (/ volume area)))

(f 3)
1
```

The general form of a `let` expression is

(let ((*variable-1* *expression-1*)
      ...
      (*variable-n* *expression-n*))
   body)

The value of the `let` expression is the value of the *body* expression in the context where the variables *variable-i* have the values of the expressions *expression-i*. The expressions *expression-i* may not refer to the variables *variable-i*.

A slight variant of the `let` expression provides a convenient way to express looping constructs. We can write a procedure that implements an alternative algorithm for computing factorials as follows:

```
(define (factorial n)
  (let fred ((count 1) (answer 1))
    (if (> count n)
        answer
        (fred (+ count 1) (* count answer)))))

(factorial 6)
720
```

Here, the symbol following the `let` (in this case `fred`) is locally defined to be a procedure that has the variables `count` and `answer` as its formal parameters. It is called the first time with the expressions 1 and 1, initializing the loop. Whenever the procedure named `fred` is called later, these variables get new values, which are the values of the operand expressions `(+ count 1)` and `(* count answer)`.

Data can be glued together to form compound data structures. A list is a data structure in which the elements are linked sequentially. A vector is a data structure in which the elements are packed in a linear array. New elements can be added to lists, but a list takes time proportional to its length to access. Vectors can be accessed in constant time, but a vector is of fixed length. All data structures in this book are implemented as combinations of lists and vectors. Compound data is constructed from components by procedures called constructors and the components are accessed by selectors.

The procedure `list` is the constructor for lists. The selector `list-ref` gets an element of the list. All selectors in Scheme are zero-based. For example,

```
(define a-list (list 37 63 49 21 88 56))

a-list
(37 63 49 21 88 56)

(list-ref a-list 3)
21

(list-ref a-list 0)
37
```

Lists are made up of pairs. A pair is made using the constructor `cons`. The selectors for the two components of the pair are `car` and `cdr`.[5] A list is a chain of pairs, such that the `car` of each pair is the list element and the `cdr` of each pair is the next pair, except for the last one, which is a distinguishable value called the empty list and which is written `()`. Thus,

```
(car a-list)
37

(cdr a-list)
(63 49 21 88 56)

(car (cdr a-list))
63

(define another-list
  (cons 32 (cdr a-list)))

another-list
(32 63 49 21 88 56)
```

[5] These names are accidents of history. They stand for "the Contents of the Address Register" and "the Contents of the Decrement Register" of the IBM 704 computer that was used for the first implementation of Lisp in the late 1950's.

```
(car (cdr another-list))
63
```

Both `a-list` and `another-list` share the same tail (their `cdr`). There is a predicate `pair?` that is true of pairs and false on all other types of data.

Vectors are simpler than lists. There is a constructor `vector` that can be used to make vectors, and there is a selector `vector-ref` for accessing the elements of a vector:

```
(define a-vector
  (vector 37 63 49 21 88 56))

a-vector
#(37 63 49 21 88 56)

(vector-ref a-vector 3)
21

(vector-ref a-vector 0)
37
```

There is a predicate `vector?` that is true of vectors and false on all other types of data. Notice that a vector is distinguished from a list on printout by the character "#" appearing before the initial parenthesis.

The elements of lists and vectors may be any kind of data, including numbers, procedures, lists, and vectors. There are numerous other procedures for manipulating list-structured data and vector-structured data that can be found in the Scheme online documentation.

Symbols are a very important kind of primitive data type that we use to make programs and algebraic expressions. You probably have noticed that the Scheme programs look just like lists. They are lists. Some of the elements of the lists that make up programs are symbols, such as "`+`" and "`vector`". If we are to make programs that can manipulate programs we need to be able to write an expression that names such a symbol. The name of the symbol "`+`" is the expression "`'+`", and in general the name of the expression "`(+ 3 a)`" is "`'(+ 3 a)`".

Thus, we can write a program to determine if an expression is a sum:

```
(define (sum? expression)
  (and (pair? expression)
       (eq? (car expression) '+)))

(sum? '(+ 3 a))
#t

(sum? '(* 3 a))
#f
```

Consider what would happen if we were to leave out the quote in the expression `(sum? '(+ 3 a))`. If the variable `a` had the value 4 we would be asking if 7 is a sum. But what we wanted to know was whether the expression "`(+ 3 a)`" is a sum. That is why we need the quote.

Bibliography

[1] IEEE Std 1178-1990, *IEEE Standard for the Scheme Programming Language,* Institute of Electrical and Electronic Engineers, Inc., New York, NY, 1991.

[2] Harold Abelson and Gerald Jay Sussman with Julie Sussman, *Structure and Interpretation of Computer Programs,* 2nd edition MIT Press and McGraw-Hill, 1996.

[3] Ralph H. Abraham and Jerrold E. Marsden, *Foundations of Mechanics,* 2nd edition, Addison-Wesley, 1978.

[4] Ralph H. Abraham, Jerrold E. Marsden, and Tudor Raţiu, *Manifolds, Tensor Analysis, and Applications,* 2nd edition, Springer Verlag, NY, 1993

[5] Church, Alonzo, *The Calculi of Lambda-Conversion* Princeton University Press, Princeton, N.J., 1941

[6] Jerrold E. Marsden, and Tudor S. Raţiu, *Introduction to Mechanics and Symmetry,* Springer Verlag, NY, 1994

[7] V. I. Arnold, *Mathematical Methods of Classical Mechanics,* Springer Verlag, NY, 1980

[8] V. I. Arnold, V. V. Kozlov, and A. I. Neishtadt, "Mathematical Aspects of Classical and Celestial Mechanics," in *Dynamical Systems III,* Springer Verlag, NY, 1988

[9] Hans Freudenthal, *Didactical Phenomenology of Mathematical Structures,* Kluwer Publishing Co., Boston, 1983.

[10] Herbert Goldstein, *Classical Mechanics,* 2nd edition, Addison-Wesley Publishing Company, 1980.

[11] Michel Hénon and Carl Heiles, Astronomical Journal, **69**, 73 (1964)

[12] E. L. Ince, *Ordinary differential equations,* Longmans, Green and Co., 1926. Reprinted by Dover, 1956.

[13] P. E. B. Jourdain, *The Principle of Least Action,* The Open Court Publishing Company, Chicago, 1913

[14] Cornelius Lanczos, *The Variational Principles of Mechanics,* 4th edition, University of Toronto Press, 1970; Dover Publications, NY, 1982.

[15] L. D. Landau and E .M. Lifshitz *Mechanics*, Third Edition, volume 1 of *Course of Theoretical Physics,* Pergamon Press, 1976.

[16] Edward Lorenz 1963.

[17] Boris V. Chirikov 1979.

[18] ???1963.

[19] *Lie Methods in Optics*, J. Sánchez Mondragón and K. B. Wolf, Editors, Springer Verlag, New York 1986, 249 p.

[20] Stanly Steinberg, *Lie series, Lie transformations, and their applications*, in [19], pp 45–103.

[21] F. R. Gantmakher, *Lektsii po analiticheskoĭ mekhanike* (Lectures on analytical mechanics), Fizmatgiz, Moscow, 1960, A barely adequate English translation by G. Yankovsky, Mir, Moscow, 1970 exists.

[22] L. D. Landau and E. M. Lifshitz, *Fluid Mechanics*, volume 6 of *Course of Theoretical Physics,* Pergamon Press, 1976.

[23] J.-M. Souriau, *Structure des systèmes dynamiques,* Dunod Université, Paris, 1970.

[24] E. T. Whittaker, *A Treatise on Analytical Dynamics,* Cambridge University Press, 1937.

[25] Richard Courant and David Hilbert, *Methods of Mathematical Physics, 2 vols.* Wiley-Interscience, New York, 1957.

[26] C. Carathéodory, *Calculus of variations and partial differential equations of the first order.* Translated by Robert B. Dean and Julius J. Brandstatter. San Francisco, Holden-Day, 1965-67.

[27] C. Carathéodory, *Geometrische Optik.* Series title: Ergebnisse der Mathematik und ihrer Grenzgebiete. 4. Bd. Berlin, J. Springer, 1937.

[28] Élie Cartan, *Leçons sur les invariants intégraux,* Hermann, Paris, 1922 (reprinted 1971)

[29] M. Born, *Vorlesungen über Atommechanik.* Berlin, J. Springer, 1925-30.

[30] L. Nordheim, *The Principles of Mechanics*, in Handbuch der Physik, vol.2 Springer, Berlin, 1927.

[31] Florian Scheck, *Mechanics,* From Newton's Laws to Deterministic Chaos, 2nd Ed. Springer-Verlag, Berlin Heidelberg New York etc., 1994

[32] Walter Thirring, *A Course in Mathematical Physics, vol.1,* Classical Dynamical Systems, Translated by Evans M. Harell. Springer-Verlag, New York Wien, 1978

[33] George Mackey, *Mathematical foundations of quantum mechanics* Benjamin, 1963

[34] Res Jost, *Poisson Brackets: and Unpedagogical Lecture* Rev. Mod. Phys. **36**, 572 (1964).

[35] Jean Dieudonné, *Treatise on Analysis, vol. I* Academic Press, NY, 1969

[36] Julius Adams Stratton, *Electromagnetic Theory,* Mc Graw Hill, New York, 1940

[37] Philip Morse and Hermann Feshbach, *Methods of Theoretical Physics,* 2 vols. Mc Graw Hill, New York, 195?

[38] Myron Bander and Claude Itzykson *The hidden symmetries of the hydrogen atom* Rev. Mod. Phys. (1965)