2

HAMILTONIAN DYNAMICS

2.1 LAGRANGIAN FORMULATION OF MECHANICS

In this section we discuss some of the basic principles of the Lagrangian formulation of classical mechanics. This provides the necessary background to learn about the Hamiltonian formulation, which, in turn, provides the natural framework in which to investigate the ideas of integrability and nonintegrability in a wide class of mechanical systems. Many of the differential equations discussed in Chapter 1 describe the motion of a particle moving in some force field (represented as the gradient of a potential energy function) and, as such, they are examples of *Newtonian equations* of motion.† Since Newton's pioneering work, the "laws" of mechanics have been the subject of ever more general and elegant formulations. General equations of motion can be seductively derived by invoking such fundamental principles as the homogeneity of space and time and the use of an almost magical variational principle ("Hamilton's principle") to the extent that the resulting "laws" would appear to have been determined from purely deductive ("absolute") principles. Nonetheless, it should always be remembered that all these results are at some point based on experimental facts and human experience—they have just stood the test of time remarkably well. (For example, there was no reason or evidence to doubt that Newton's laws could describe microscopic systems until spectroscopic evidence came along to indicate the need for quantum mechanics.)

†The reader is assumed to be familiar with the basics of Newtonian mechanics and such concepts as constraints and generalized coordinates (see, for example, Chapter I of Goldstein (1980)).

2.1.a The Lagrangian Function and Hamilton's Principle

If one considers a mechanical system consisting of a collection of particles—interacting amongst each other according to well-defined force laws—then experience has shown that the "state of the system" is completely described by the set of all the positions and velocities of the particles. The coordinate frame need not be cartesian, as was the case in Newton's work, and the description can be effected by means of some set of "generalized coordinates" q_i $(i = 1, \ldots, n)$ and "generalized velocities" $\dot{q}_i$ $(i = 1, \ldots, n)$. (The use of generalized coordinates relieves a system from the explicit presence of holonomic constraints.)

If a system moves from a position at some time t_1, labelled by the coordinate set $\mathbf{q}^{(1)} = q_1(t_1), \ldots, q_n(t_1)$, to a position $\mathbf{q}^{(2)} = q_1(t_2), \ldots, q_n(t_2)$ at another time t_2, then the actual motion can be determined from Hamilton's principle of least action. This requires that the integral of the so-called *Lagrangian* function takes the minimum possible value between the initial and final times. For the moment, we treat the Lagrangian as a "black box", merely stating that it can only be some function of those variables on which the state of a system can depend (i.e., the generalized coordinates, velocities, and time), namely,

$$L = L(q_1, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n, t) \tag{2.1.1}$$

The famous "principle of least action," or "Hamilton's principle," requires that the *action integral*

$$W = \int_{t_1}^{t_2} L(\mathbf{q}, \dot{\mathbf{q}}, t)\, dt \tag{2.1.2}$$

be a minimum. For the moment, we drop the subscript on the q_i's and $\dot{q}_i$'s and assume a single degree of freedom. The positions $q^{(1)}$ and $q^{(2)}$ at the initial and final times t_1 and t_2 are assumed fixed. (Allowing the end points to also vary with time has other important consequences.) There can be many different paths $q(t)$ connecting $q^{(1)}$ and $q^{(2)}$, and the aim is to find those that *extremize* (which usually means minimize but can, in fact, also result in a maximum) the action (2.1.2). This is done by looking at the effect of a "first variation," that is, adding small excursions along the path which vanish at either end (i.e., $\delta q(t_1) = \delta q(t_2) = 0$). A remarkable feature of this procedure is that we are considering the effect of these variations about a path which we do not yet know. The first variation of the action W is then determined by

$$\delta W = \int_{t_1}^{t_2} L(q + \delta q, \dot{q} + \delta \dot{q}, t)\, dt - \int_{t_1}^{t_2} L(q, \dot{q}, t)\, dt \tag{2.1.3}$$

By expanding the first integrand to first order, one obtains the variation

$$\delta W = \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q}\, \delta q + \frac{\partial L}{\partial \dot{q}}\, \delta \dot{q} \right) dt \tag{2.1.4}$$

Using $\delta \dot{q} = d\delta q/dt$ and integrating the second term by parts yields

$$\delta W = \left| \frac{\partial L}{\partial \dot{q}}\, \delta q \right|_{t_1}^{t_2} + \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}} \right) \right) \delta q\, dt \tag{2.1.5}$$

By the end-point condition, the first term on the right-hand side vanishes. If the variation is to be an extremum, then $\delta W = 0$; this can only occur if the integrand vanishes, that is,

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}} \right) = 0 \tag{2.1.6}$$

For n degrees of freedom $q_1, \ldots, q_n$, the variation must be effected for each variable independently, that is, $q_i(t) + \delta q_i(t)$. The net result is the set of equations

LAGRANGE'S EQUATIONS

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i} \right) - \frac{\partial L}{\partial q_i} = 0 \tag{2.1.7}$$

which are the celebrated *Lagrange's equations*. If the (correct!) form of the Lagrangian is known for the given mechanical system, then the set of second-order equations (2.1.7) are the equations of motion for the system and, given the initial data $q_i(0)$, $\dot{q}_i(0)$ $(i = 1, \ldots, n)$ will determine the entire history of the system.†

In determining the correct form for the Lagrangian function it is interesting to see how far one can go in making this choice by invoking only the most basic principles. In their brilliant text on mechanics, Landau and Lifshitz (1960) persuasively argue that, for a free particle at least, the principles of homogeneity of time and isotropy of space‡ determine that the Lagrangian can only be proportional to the square of the (generalized) velocities. If the constant of proportionality is taken to be half the particle mass, then the Lagrangian for a system of noninteracting particles is just their total kinetic energy in rectilinear coordinates, that is,

FREE PARTICLE

†So powerful did this deterministic framework appear that Laplace was led to say "We ought then to regard the present state of the universe as the effect of its preceeding state and as the cause of its succeeding state."

‡These two properties ensure that the motion can be considered in the context of an "inertial frame," that is, independent of its "absolute" position in space and time.

$$L = T = \sum_{i=1}^{n} \frac{1}{2} m_i \dot{q}_i^2$$

Beyond this, "experimental" facts have to be invoked in that if the particles interact amongst each other according to some force law contained in a "potential energy function" $V(q_1, \ldots, q_n)$, then, to quote Landau and Lifshitz (1960), "experience has shown that" the correct form of the Lagrangian is

$$L = T - V = \sum_{i=1}^{n} \tfrac{1}{2} m_i \dot{q}_i^2 - V(q_1, \ldots, q_n) \tag{2.1.8}$$

The potential energy function is such that the force acting on each particle is determined by

$$F_i = -\frac{\partial}{\partial q_i} V(q_1, \ldots, q_n) \tag{2.1.9}$$

(This provides a definition of the potential energy, since it ensures that the net work done by a system in traversing a closed path in the configuration (i.e., coordinate) space is zero.) For velocity-independent potentials, Lagrange's equations (Eqs. (2.1.7)) become

NEWTON'S EQUATION $\longrightarrow$

$$m\ddot{q}_i = -\frac{\partial V}{\partial q_i} \tag{2.1.10}$$

which, in the case of cartesian coordinates, are just Newton's equations.

2.1.b Properties of the Lagrangian

Given the Lagrangian for a system of (interacting) particles, a number of interesting properties of that system can be deduced. First we consider the total time derivative of the Lagrangian, that is,

$$\begin{aligned} \frac{d}{dt} L(q, \dot{q}, t) &= \sum_i \frac{\partial L}{\partial q_i} \dot{q}_i + \sum_i \frac{\partial L}{\partial \dot{q}_i} \ddot{q}_i + \frac{\partial L}{\partial t} \\ &= \sum_i \frac{d}{dt}\left(\dot{q}_i \frac{\partial L}{\partial \dot{q}_i} \right) + \frac{\partial L}{\partial t} \end{aligned}$$

Thus

$$\frac{d}{dt}\left(\sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L \right) = -\frac{\partial L}{\partial t} \tag{2.1.11}$$

For a closed system (i.e., one which does not interact with any external forces), the homogeneity of time ensures that L does not depend explicitly on time, and thus the "energy"

$$E = \sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L \tag{2.1.12}$$

is a constant of the motion; that is, the system considered is conservative (see Chapter 1). Furthermore, using the definition of L in (2.1.8), it is easily deduced that

$$E = T + V \tag{2.1.13}$$

Using L, one may define the generalized forces

$$F_i = \frac{\partial L}{\partial q_i} \tag{2.1.14}$$

and, most importantly, the *generalized momenta*

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \tag{2.1.15}$$

where only for cartesian coordinates do we obtain $p_i = m\dot{q}_i$. With these two definitions, Lagrange's equations can then be cast in the form

$$\dot{p}_i = F_i, \qquad i = 1, \ldots, n \tag{2.1.16}$$

Clearly, if any one of the generalized coordinates, say q_k, is missing from the Lagrangian, we obtain the associated generalized force $F_k = 0$ and hence (from (2.1.6)) the corresponding generalized momentum p_k =constant. Missing coordinates are sometimes referred to as *cyclic*—clearly, cyclic coordinates simplify the integration of the equations of motion. With the above definition of the p_i, the energy of the system (2.1.12) can then be written as

$$E = \sum_{i=1}^{n} p_i \dot{q}_i - L \tag{2.1.17}$$

If a system is closed and space is homogeneous, then the net effect of all the particle forces must be zero, that is, $\sum_{i=1}^{n} F_i = 0$ (in Newton's third law this is stated, for two bodies, as "action and reaction are equal and opposite"). In this case we may deduce from (2.1.16) that $\sum_{i=1}^{n} p_i =$ constant; that is, the overall translation of a system of particles is constant.

Thus we see that by invoking such fundamental principles as homogeneity of time and space (for closed systems), one may deduce basic conservation laws such as the conservation of energy and total momentum. These results are examples of a deep and general result known as *Noether's theorem*, which states that for every group of transformations that leaves the Lagrangian function invariant, there is an associated conserved quantity; for example, invariance under translation in time and space leads to conservation of energy and (linear) momentum, respectively. Another simple example is a system invariant under rotation—here angular momentum will be conserved.

NOETHER'S THEOREM

2.1.c Properties of the Generalized Momenta

In the Lagrangian picture of mechanics, the generalized coordinates and velocities are considered as independent variables. Now we have also defined another set of variables, the generalized momenta p_i (Eq. (2.1.15)). The simple connection between the generalized momenta and velocities in the cartesian coordinate system is deceptive in that the p_i are truly a completely independent (from the q_i and $\dot{q}_i$) set of variables. The differences are deep and are most clearly seen when viewed from a more geometric point of view.† So deep and elegant is this structure that Arnold (1978) has described Hamiltonian mechanics (i.e., the description of mechanics in terms of the p_i and q_i) as "geometry in phase space."

In a more traditional framework, an important property of the p_i that distinguishes them from the q_i is that they are expressible as the gradient of a scalar field—this is a simple way of demonstrating their covariant properties. To see this, we return to the action integral (2.1.2). For a given extremal path, that is, a path satisfying Eqs. (2.1.7), this is just a definite integral, that is, the value of the action along the path connecting $q(t_1)$ and $q(t_2)$. A variational principle can still be applied to (2.1.2)—but this time to see how the action varies between neighboring extremal paths with the same initial point but different final points. So now one looks at the variation of W for $q = q(t) + \delta q$, where $q(t)$ is an actual extremal path with $q^{(1)} = q(t_1)$ fixed and $q^{(2)} = q(t_2) + \delta q(t_2)$ as the varying end point. The

†The velocities are examples of tangent vectors and transform as *contravariant* variables. The combined set of variables q_i, $\dot{q}_i$ $(i = 1, \ldots, n)$ forms a $2n$-dimensional manifold known as a *tangent bundle* (TM), and the Lagrangian then becomes the mapping of the tangent-bundle space to a scalar field, namely, $L: TM \rightarrow R$ (i.e., it converts the set q_i, $\dot{q}_i$ to a real number). Momenta have completely different geometric properties. They transform as *covariant* variables, and the *phase space* made up of the set q_i, p_i $(i = 1, \ldots, n)$ is a $2n$-dimensional *symplectic* manifold with very different geometric properties from the tangent bundle space of Lagrangian mechanics. For a full account, the reader is referred to V. I. Arnold's (1978) wonderful book *Mathematical Methods of Classical Mechanics*. An introductory account of these concepts is given in Appendix 2.2.

variation leads to the same result as (2.1.5), that is,

$$\delta W = \left|\frac{\partial L}{\partial \dot{q}}\,\delta q\right|_{t_1}^{t_2} + \int_{t_1}^{t_2}\left(\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right)\right)\delta q\, dt \tag{2.1.18}$$

but since the path is assumed to be extremal, the integral vanishes and one is left with just the end-point contributions. Since the initial point is fixed, we have $\delta q(t_1) = 0$; and denoting $\delta q(t_2)$ as just δq and using $p = \partial L/\partial \dot{q}$, one has $\delta W = p\,\delta q$ or

$$\delta W = \sum_{i=1}^{n} p_i\,\delta q_i \tag{2.1.19}$$

for a system of n degrees of freedom. From this result follows the property that the p_i are *gradients of the action*, that is,

$$p_i = \frac{\partial W}{\partial q_i} \tag{2.1.20}$$

at a given time along a given extremal path. By contrast, note that it is not possible to express $\dot{q}$ as the gradient of a scalar field.

2.2 HAMILTONIAN FORMULATION OF MECHANICS

Hamiltonian mechanics is the description of a mechanical system in terms of generalized coordinates q_i and generalized momenta p_i. Although the Hamiltonian formulation of classical mechanics contains the same physical information as the Lagrangian picture, it is far better suited for the formulation of quantum mechanics, statistical mechanics, and perturbation theory. In particular, the use of Hamiltonian phase space provides the ideal framework for a discussion of the concepts of integrability and nonintegrability and the description of the chaotic phenomena that can be exhibited by nonintegrable systems.

2.2.a Transformation to the Hamiltonian Picture

To effect the transformation from the Lagrangian description involving the q_i and the $\dot{q}_i$ to the Hamiltonian description, one uses the standard technique of Legendre's transformation (see Appendix 2.1). The Legendre transform of $L = L(\mathbf{q}, \dot{\mathbf{q}}, t)$ with respect to $\dot{\mathbf{q}}$ to a new function in which $\dot{\mathbf{q}}$ is expressed in terms of $\mathbf{p}$ is

$$H(\mathbf{p}, \mathbf{q}, t) = \sum_{i=1}^{n} p_i\dot{q}_i - L(\mathbf{q}, \dot{\mathbf{q}}, t) \tag{2.2.1}$$

where $\mathbf{p}$, $\mathbf{q}$, and $\dot{\mathbf{q}}$ are the n-component vectors $\mathbf{p} = (p_1, \ldots, p_n)$, $\mathbf{q} = (q_1, \ldots, q_n)$, $\dot{\mathbf{q}} = (\dot{q}_1, \ldots, \dot{q}_n)$ and the new function H is the *Hamiltonian* of the system. The crucial relationship is that which defines p_i in terms of the q_i and $\dot{q}_i$, namely,

$$p_i(\mathbf{q}, \dot{\mathbf{q}}, t) = \frac{\partial L}{\partial \dot{q}_i}(\mathbf{q}, \dot{\mathbf{q}}, t) \tag{2.2.2}$$

which, providing

$$\det\left|\frac{\partial^2 L}{\partial \dot{q}_i \, \partial \dot{q}_j}\right| \neq 0 \tag{2.2.3}$$

can be inverted to express the $\dot{q}_i$ in terms of the p_i with (at this stage) q_i and t treated as parameters. As a simple example of this transformation, consider the Lagrangian

$$L = \sum_{i=1}^{n} \frac{1}{2} m_i \dot{q}_i^2 - V(q_1, \ldots, q_n) \tag{2.2.4}$$

From this we determine

$$p_i = \frac{\partial L}{\partial \dot{q}_i} = m\dot{q}_1 \tag{2.2.5}$$

and since condition (2.2.3) is satisfied, the inverse is (trivially in this case)

$$\dot{q}_i = \frac{p_i}{m_i} \tag{2.2.6}$$

and thus the Hamiltonian is

$$\begin{aligned} H(\mathbf{p}, \mathbf{q}) &= \sum_{i=1}^{n} p_i\left(\frac{p_i}{m_i}\right) - \left\{\sum_{i=1}^{n} \frac{1}{2} m_i \left(\frac{p_i}{m_i}\right)^2 - V(q_1, \ldots, q_n)\right\} \\ &= \sum_{i=1}^{n} \frac{1}{2m_i} p_i^2 + V(q_1, \ldots, q_n) \end{aligned} \tag{2.2.7}$$

Although the Lagrangian (2.2.4) describes an important class of mechanical system, the simplicity of the relationship between the p_i and $\dot{q}_i$ is such that some of the subtlety is lost. A standard example of a less trivial transformation is provided by the case of a particle moving under gravity but constrained to a smooth wire frame of specified shape.†

†This is an example of an holonomic constraint.

Consider a bead of mass m sliding smoothly on a wire of shape $z = f(x)$ in the vertical (z, x)-plane. To begin with, think of unconstrained motion in this plane. This will require, in the Lagrangian description, two coordinates and velocities (i.e., x, z and $\dot{x}$, $\dot{z}$); thus the kinetic energy is $T = \frac{1}{2}\, m(\dot{x}^2 + \dot{z}^2)$. Now introduce the relationship between x and z, that is, $z = f(x)$, from which one obtains $\dot{z} = \dot{x}(df/dx) \equiv \dot{x}f'(x)$. Thus one finds

$$T = \tfrac{1}{2}m(\dot{x}^2 + \dot{z}^2) = \tfrac{1}{2}m\dot{x}^2(1 + (f'(x))^2) \tag{2.2.8}$$

The potential energy is just that due to gravity (i.e., $V = mgz = mgf(x)$), and so the Lagrangian is

$$L = \tfrac{1}{2}m\dot{x}^2[1 + (f'(x))^2] - mgf(x) \tag{2.2.9}$$

From Eq. (2.1.5) the generalized momentum is

$$p = \frac{\partial L}{\partial \dot{x}} = m\dot{x}(1 + (f'(x))^2) \tag{2.2.10}$$

and hence

$$\dot{x} = \frac{p}{m(1 + (f'(x))^2)} \tag{2.2.11}$$

Thus from (2.2.1) the Hamiltonian is

$$H(p, x) = p\,\frac{p}{m(1 + (f'(x))^2)} - \left\{\left(\frac{m}{2}\right)\frac{p^2}{m^2(1 + (f'(x))^2)^2}(1 + (f'(x))^2) - mgf(x)\right\}$$

$$= \frac{p^2}{2m(1 + (f'(x))^2)} + mgf(x) \tag{2.2.12}$$

2.2.b Hamilton's Equations

Given the Lagrangian for a system, Lagrange's equations of motion were derived from Hamilton's principle. Clearly, we now want to derive equations of motion for the Hamiltonian formulations of the problem. These can also be derived on the basis of a variational principle (see Section 2.3.c for a discussion of this) but are more directly seen as follows. The differential of H, defined by (2.2.1), is

$$dH = \sum_i p_i\, d\dot{q}_i + \dot{q}_i\, dp_i - \frac{\partial L}{\partial \dot{q}_i}\, d\dot{q}_i - \frac{\partial L}{\partial q_i}\, dq_i - \frac{\partial L}{\partial t}\, dt \tag{2.2.13}$$

The first and third terms on the right-hand side cancel by the definition $p_i = \partial L/\partial \dot{q}_1$; and using the relation $\dot{p}_i = \partial L/\partial q_i$ (Eq. (2.1.6)), one obtains

$$dH = \sum \dot{q}_1\, dp_i - \dot{p}_i\, dq_i - \frac{\partial L}{\partial t}\, dt \tag{2.2.14}$$

Thus one obtains the famous "canonical" or *Hamiltonian equations* of motion, namely,

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i} \tag{2.2.15}$$

plus the additional relationship† (for explicitly time-dependent systems)

$$\frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t} \tag{2.2.16}$$

The system of equations (2.2.15) form a set of $2n$ first-order equations in contrast to the set of n second-order equations obtained in the Lagrangian description. Although in Chapter 1 we saw that a second-order equation, say of the form $\ddot{x} = f(x)$, could be written as a pair of first-order equations by introducing a new variable $y = \dot{x}$, it should be clear that they are not necessarily in Hamiltonian form. Consider the sliding-bead problem. Hamilton's equations are

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m(1 + (f'(x))^2)} \tag{2.2.17a}$$

$$\dot{p} = -\frac{\partial H}{\partial x} = \frac{p^2 f'(x) f''(x)}{m(1 + (f'(x))^2)^2} - mgf'(x) \tag{2.2.17b}$$

On the other hand, Lagrange's equation is

$$\ddot{x} = -\frac{f'(x)(\dot{x}^2 f''(x) + g)}{1 + (f'(x))^2} \tag{2.2.18}$$

Introducing the variable $y = \dot{x}$, one obtains the pair

$$\dot{x} = y \tag{2.2.19a}$$

$$\dot{y} = -\frac{f'(y^2 f'' + g)}{1 + (f')^2} \tag{2.2.19b}$$

which are clearly quite different from the pair (2.2.17a) and (2.2.17b).

†In addition, one may easily demonstrate that $dH/dt = \partial H/\partial t$. Comparison with the canonical equations (2.2.15) suggests that, formally, one could also consider $-H$ and t to be a pair of canonical variables. This concept is especially valuable for time-dependent Hamiltonians where one often considers the $(2n+2)$–dimensional "extended" phase space of $p_1, \ldots, p_n, q_1, \ldots, q_n; -H, t$. (See the later discussion of the Poincaré–Cartan invariant.)

Hamilton's equations (2.2.15) have a number of important properties; for the moment, we discuss them in the context of a time-independent Hamiltonian. First of all, the set of $2n$ variables $q_1, \ldots, q_n, p_1, \ldots, p_n$—often called the "canonical" or "canonically conjugate" variables (e.g., "p_i is the momentum conjugate to q_i")—define a $2n$-dimensional *phase space* (cf. the discussion of phase space in Chapter 1). The solution to Hamilton's equations

$$q_i(t) = q_i(\mathbf{q}_0, \mathbf{p}_0, t), \qquad p_i(t) = p_i(\mathbf{q}_0, \mathbf{p}_0, t) \tag{2.2.20}$$

where $\mathbf{q}_0 = (q_1(0), \ldots, q_n(0))$, $\mathbf{p}_0 = (p_1(0), \ldots, p_n(0))$ are the set of initial conditions, define the mechanical state of the system at time t. As time evolves, $\mathbf{q}(t)$, $\mathbf{p}(t)$ map out a phase-space trajectory which explores certain regions of the phase space. Precisely what regions these are is *the* fundamental issue—which we shall soon discuss.

It is easy to see that Eqs. (2.2.15) satisfy the "incompressibility" condition

$$\sum_{i=1}^{n} \left(\frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i} \right) = 0 \tag{2.2.21}$$

Imagine a blob of phase-space "fluid"—Eq. (2.2.21) is just a statement that this blob has zero divergence. Thus a volume element in phase space is preserved under the Hamiltonian flow—this is *Liouville's theorem* and is one of the most fundamental properties of Hamiltonian systems.† In the sliding-bead problem, for example, it is easily seen from Eqs. (2.2.17) that the phase-space flow is indeed divergenceless. Notice on the other hand that the pair (2.2.19) deduced from the Lagrangian does not preserve volume (area, to be more precise, in this case) in the (x, y) "phase space."

So symmetric are Hamilton's equation in p and q that it seems natural to consider the variables p_i and q_i on very much of an equal footing. Often it is convenient to introduce a single "set" of $2n$ coordinates z_i, where $\mathbf{z} = (q_i, \ldots, q_n, p_i, \ldots, p_n)$. Thus for a given Hamiltonian $H = H(\mathbf{q}, \mathbf{p}) = H(\mathbf{z})$, Hamilton's equations can be written in the concise form

$$\dot{\mathbf{z}} = \mathbf{J} \cdot \nabla H(\mathbf{z}) \tag{2.2.22}$$

where $\nabla = (\partial z_1, \ldots, \partial z_{2n})$ and the $2n \times 2n$ matrix $\mathbf{J}$ is termed the *symplectic* matrix

$$\mathbf{J} = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix} \tag{2.2.23}$$

where $\mathbb{1}$ is the $n \times n$ unit matrix.

†A more geometric account of Liouville's theorem is given in Appendix 2.2.

2.2.c Poisson Brackets*

Of particular importance is our ability to integrate Hamilton's equations. For systems with just one degree of freedom (i.e., just a single pair of canonical variables (p, q)), we can integrate the pair of first-order equations in the ways discussed in Chapter 1. However, whether it be one or many degrees of freedom, the crucial step is to identify the integrals of motion. In the Hamiltonian picture, the time dependence of dynamical quantities can be formulated very elegantly. Consider some function $f = f(p, q, t)$; then

$$\begin{aligned}\frac{df}{dt} &= \sum_{i=1}^{n}\left(\frac{dq_i}{dt}\frac{\partial f}{\partial q_i}+\frac{dp_i}{dt}\frac{\partial f}{\partial p_i}\right)+\frac{\partial f}{\partial t}\\ &= \sum_{i=1}^{n}\left(\frac{\partial H}{\partial p_i}\frac{\partial f}{\partial q_i}-\frac{\partial H}{\partial q_i}\frac{\partial f}{\partial p_i}\right)+\frac{\partial f}{\partial t}\\ &= [H, f]+\frac{\partial f}{\partial t}\end{aligned} \tag{2.2.24}$$

where $[H, f]$ is the *Poisson bracket* of f with H. There is a close analogy between the Poisson brackets of classical mechanics and the commutator brackets of quantum mechanics. In fact, one can write the Poisson bracket for any pair of dynamical quantities, for example,

$$[g, f] = \sum_{i=1}^{n}\left(\frac{\partial g}{\partial p_i}\frac{\partial f}{\partial q_i}-\frac{\partial g}{\partial q_i}\frac{\partial f}{\partial p_i}\right) \tag{2.2.25}$$

If a quantity is explicitly time independent (i.e., $f = f(p, q)$ and its Poisson bracket with H vanishes), then it is clear from (2.2.24) that f is a constant of motion. Obviously, since the Poisson bracket of H with itself is zero, the energy of a time-independent system (i.e., $H = E$) is a constant of motion.

Following from its definition (Eq. (2.2.25)), the Poisson bracket may be shown to have a variety of properties. For the three given functions f, g, h, one finds

$$[f, g] = -[g, f] \tag{2.2.26a}$$

$$[f+g, h] = [f, h]+[g, h] \tag{2.2.26b}$$

$$[fg, h] = f[g, h]+g[f, h] \tag{2.2.26c}$$

$$[f,[g, h]]+[g,[h, f]]+[h,[f, g]] = 0 \tag{2.2.26d}$$

the last of which, with its characteristic cyclic structure, is known as *Jacobi's identity*. The set of properties (2.2.26) shows that the Poisson brackets satisfy what is known as a *Lie algebra*. There is nothing to stop one from choosing the various functions f, g, h to be just individual canonical

variables, in which case one obtains relations of the form

$$[q_i, q_j] = 0, \qquad [p_i, p_j] = 0, \qquad [p_i, q_j] = \delta_{ij} \tag{2.2.27}$$

which are closely analogous to those obtained in quantum mechanics (e.g., the third relation becomes $[\hat{p}_i, \hat{q}_j] = -i\hbar\delta_{ij}$). If f and g are both constants of motion (i.e., $[H, f] = [H, g] = 0$), then it follows by Poisson's theorem that the bracket between f and g is also a constant of motion, that is, $[f, g] =$ constant. This is easily seen from the Jacobi identity (2.2.26d), that is, $[f,[g, H]]+[g,[H, f]]+[H,[f, g]] = 0$. Since the first two brackets vanish (because f and g are constants), we are immediately left with the desired result $[H,[f, g]] = 0$, which indicates that $[f, g]$ is also a constant. However, Poisson's theorem may not always be very useful in practice (i.e., for constructing new integrals of motion), since the bracket $[f, g]$ may just be a simple constant (e.g., zero) or just a function of the original integrals f and g.

In Chapter 1 we saw that, in general, a system of n first-order equations requires $n-1$ integrals (these include both the nontrivial "integrals of motion" and the trivial "constants of integration") in order to effect a complete "integration." Does this mean, then, that for the system of $2n$ equations of a Hamiltonian system we require $2n-1$ integrals of motion to solve the problem? Fortunately, as already mentioned, it turns out that, owing to the special symplectic structure of Hamilton's equations, one only requires n integrals of motion. However, to see how this miracle occurs, it is useful to first of all learn about what are termed *canonical transformations*. These are the transformations of variables for which the Hamiltonian structure of the system is still preserved.

2.3 CANONICAL TRANSFORMATIONS

In the Lagrangian description of a system (i.e., the description in terms of generalized coordinates and velocities q_i, $\dot{q}_i$), it is sometimes convenient to transform to some new set of generalized coordinates, that is,

$$Q_i = Q_i(q_1, \ldots, q_n) \tag{2.3.1}$$

to simplify the integration of the equations of motion (e.g., a transformation from cartesian to polar coordinates). In the Hamiltonian description, there are now two sets of independent variables, the p_i and q_i $(i = 1, \ldots, n)$, which, as we have discussed, are very much on an equal footing. Thus we now have to consider the possibility of transformations from one set of phase-space variables (p_i, q_i) to some new set (P_i, Q_i), that is,

$$\begin{aligned} P_i &= P_i(q_1, \ldots, q_n, p_1, \ldots, p_n) \\ Q_i &= Q_i(q_1, \ldots, q_n, p_1, \ldots, p_n) \end{aligned} \tag{2.3.2}$$

Notice that the new P_i and Q_i can be, in general, functions of both the old p_i and q_i. Those cases in which the transformations just involve making the new P_i and Q_i functions of only the old p_i and q_i, respectively (i.e., as in Eq. (2.3.1)), are referred to as *point transformations*. Transformations of the form (2.3.2) are referred to as *canonical transformations* if the symplectic structure of the system is still preserved. Loosely speaking (a more precise, geometric definition will be given later), this means that the canonical form of Hamilton's equations are still preserved, that is,

$$\dot{Q}_i = \frac{\partial}{\partial P_i} H'(\mathbf{Q}, \mathbf{P}), \qquad \dot{P}_i = -\frac{\partial}{\partial Q_i} H'(\mathbf{Q}, \mathbf{P}) \tag{2.3.3}$$

where $H' = H'(\mathbf{Q}(\mathbf{q}, \mathbf{p}), \mathbf{P}(\mathbf{q}, \mathbf{p}))$ is the transformed Hamiltonian. (The transformation of $H(\mathbf{p}, \mathbf{q})$ to $H'(\mathbf{P}, \mathbf{Q})$ is not always just a simple substitution of variables—see later.)

2.3.a The Preservation of Phase Volume

A fundamental property of canonical transformations is that phase volume is preserved.† If $\prod_{i=1}^{n} dp_i\, dq_i$ represents a volume element in the "old" phase space and $\prod_{i=1}^{n} dP_i\, dQ_i$ represents a volume element in the "new" phase space, then we require that

$$\int \prod_{i=1}^{n} dp_i\, dq_i = \int \prod_{i=1}^{n} dP_i\, dQ_i \tag{2.3.4}$$

where the integral sign represents a $2n$-dimensional integration over a

†In fact, the preservation of phase volume is just one of a hierarchy of quantities, preserved under canonical transformation, known as the Poincaré invariants. The first of these is the invariant

$$\int\int \sum_{i=1}^{n} dp_i dq_i = \iint \sum_{i=1}^{n} dP_i dQ_i$$

which represents the sum of areas (of a phase-space element) projected onto the set of (p_i, q_i) planes. In geometric language this is expressed in terms of the "*differential 2-form*," that is,

$$\sum_{i=1}^{n} dp_i \wedge dq_i = \sum_{i=1}^{n} dP_i \wedge dQ_i$$

where $\wedge$ denotes the so called wedge product. This result provides a rigorous, geometric definition of canonical transformations. All other invariances, including (2.3.4), follow from this (see Appendix 2.2).

prescribed volume in phase space. The two integrals are related by the Jacobian of transformation, that is,

$$\int \prod_{i=1}^{n} dP_i\, dQ_i = \int \frac{\partial(P_1, \ldots, P_n, Q_1, \ldots, Q_n)}{\partial(p_1, \ldots, p_n, q_1, \ldots, q_n)} \prod_{i=1}^{n} dp_i\, dq_i \qquad (2.3.5)$$

Thus a volume preserving transformation must have unit Jacobian, namely,

$$\frac{\partial(P_1, \ldots, P_n, Q_1, \ldots, Q_n)}{\partial(p_1, \ldots, p_n, q_1, \ldots, q_n)} = \frac{\partial(p_1, \ldots, p_n, q_1, \ldots, q_n)}{\partial(P_1, \ldots, P_n, Q_1, \ldots, Q_n)} = 1 \qquad (2.3.6)$$

Consider the very simple example

$$Q = -p, \qquad P = q \qquad (2.3.7)$$

Then

$$\frac{\partial(P, Q)}{\partial(p, q)} = \begin{vmatrix} \dfrac{\partial P}{\partial p} & \dfrac{\partial Q}{\partial p} \\ \dfrac{\partial P}{\partial q} & \dfrac{\partial Q}{\partial q} \end{vmatrix} = \begin{vmatrix} 0 & -1 \\ 1 & 0 \end{vmatrix} = 1 \qquad (2.3.8)$$

which therefore shows that (2.3.7) is a volume-preserving (canonical) transformation. The transformation (2.3.7) demonstrates on just how equal a footing the p and q are; that is, they can be interchanged—but with a sign change. Notice that if we did not make that sign change (e.g., $Q = p$, $P = q$), the Jacobian would be -1. In fact, this need for the sign change should not be surprising since it is required to preserve the form of Hamilton's equations (2.3.3) under interchange of P and Q.

An example of a noncanonical transformation is that from polar to cartesian coordinates, that is,

$$q = P \cos Q, \qquad p = P \sin Q \qquad (2.3.9)$$

since

$$\frac{\partial(q, p)}{\partial(Q, P)} = \begin{vmatrix} -P \sin Q & P \cos Q \\ \cos Q & \sin Q \end{vmatrix} = -P \qquad (2.3.10)$$

which indicates that phase volume is not preserved.

Liouville's theorem is the statement that phase volume is preserved under the Hamiltonian flow—we saw this in Section 2.2.b as an almost obvious "incompressibility condition" that follows from the form of Hamilton's equations. In fact, we can couch Liouville's theorem in the language of canonical transformations as follows. Consider some phase-space tra-

jectory along which some initial q_0, p_0 at time t_0 evolve to some q_1, p_1 at a (short) time t later, that is,

$$q_1 = q(t+\delta t) \doteq q_0 + \delta t \left.\frac{dq}{dt}\right|_{t=t_0} + O(\delta t^2)$$

$$= q_0 + \delta t \frac{\partial}{\partial p_0} H(q_0, p_0, t) + O(\delta t^2)$$

$$p_1 = p(t+\delta t) = p_0 + \delta t \left.\frac{dp}{dt}\right|_{t=t_0} + O(\delta t^2)$$

$$= p_0 - \delta t \frac{\partial}{\partial q_0} H(q_0 p_0, t) + O(\delta t^2)$$

If the transformations from q_0, p_0 to q_1, p_1 is, in fact, a canonical transformation from one set of variables to the other, then the Jacobian $\partial(q_1, p_1)/\partial(q_0, p_0)$ must be unity. We find

$$\frac{\partial(q_1, p_1)}{\partial(q_0, p_0)} = \begin{vmatrix} \dfrac{\partial q_1}{\partial q_0} & \dfrac{\partial p_1}{\partial q_0} \\ \dfrac{\partial q_1}{\partial p_0} & \dfrac{\partial p_1}{\partial p_0} \end{vmatrix} = \begin{vmatrix} 1 + \delta t \dfrac{\partial^2 H}{\partial q_0 \, \partial p_0} & -\delta t \dfrac{\partial^2 H}{\partial q_0^2} \\ \delta t \dfrac{\partial^2 H}{\partial p_0^2} & 1 - \delta t \dfrac{\partial^2 H}{\partial q_0 \, \partial p_0} \end{vmatrix}$$

$$= 1 + O(\delta t^2)$$

$$= 1 \quad \text{in} \quad \lim \delta t \to 0$$

Note that the vanishing term is $O(\delta t^2)$ rather than $O(\delta t)$. Because this change is proportional to $O(\delta t^2)$, it follows that over any finite period of time (i.e., any multiple of δt), the total change of area goes as $O(\delta t)$—which vanishes in the limit $\delta t \to 0$. Thus the "infinitesimal transformation" generated by the Hamiltonian itself is a canonical transformation. The phase volume in the variables q_0, p_0 is preserved under transformation (due to the Hamiltonian flow) to the "new" variables q_1, p_1—which is, of course, just a statement of Liouville's Theorem.

2.3.b The Optimal Transformation

The practical use of canonical transformations (although they certainly have an elegant structure in their own right) is to find those transformations

that make the integration of Hamilton's equations as simple as possible. The optimal case is the one in which all the Q_i are cyclic; that is, the transformed Hamiltonian depends only on the new momenta P_i:

$$H(p_1, \ldots, p_n, q_1, \ldots, q_n) \longrightarrow H'(P_1, \ldots, P_n) \tag{2.3.11}$$

Hamilton's equation then becomes very simple since

$$\dot{P}_i = -\frac{\partial H'}{\partial Q_i} = 0, \qquad \text{i.e., } P_i = \text{const.}, \quad i = 1, \ldots, n \tag{2.3.12a}$$

$$\dot{Q}_i = \frac{\partial H'}{\partial P_i} = f_i(P_i, \ldots, P_n) \tag{2.3.12b}$$

where the f_i are some time-independent function of the P_i. The equation for Q_i can then be immediately integrated, that is,

$$Q_i = f_i t + \delta_i, \qquad i = 1, \ldots, n \tag{2.3.12c}$$

where $\delta_i = Q_i(0)$ are a set of arbitrary constants determined by the initial conditions. Clearly, the new set of "momenta" P_i are constants of the motion. Thus if we can find them we are able to effect a complete integration of the equations of motion. The P_i and δ_i constitute a set of $2n$ integrals. The n P_i are the set of nontrivial constants of motion (or first integrals) that enable one to "perform" the integration, and the n δ_i are the set of trivial constants of integration that enable one to "complete" the integration. (If need be, these solutions can then be transformed back, in principle at least, to the original representation in terms of "old" p_i's and q_i's.) Of course we have to be able to do two things: (1) find these magical new variables and (2) know how to correctly transform the Hamiltonian into its new representation.

2.3.c Generating Functions

Canonical transformations are effected by means of so-called *generating functions*.† One way to introduce them is through a variational principle. Although formally elegant, it is perhaps easier, at least for time-independent problems, to proceed via a simpler route that only involves the principle of phase-volume preservation. (Here we follow the presentation of

†It is important to emphasize that generating functions are more than formalism—as sometimes appears on a first reading. They are extremely useful. They enable one to find, directly, both the "new" canonical P and Q and their relationship to the "old" p and q. This is, in effect, "two for the price of one." If one did not use a generating function but just started off with some $Q = Q(q, p)$, one would probably have to work quite hard to find the corresponding canonical $P = P(q, p)$.