Chapter Fourteen

Hamilton's equations and phase space

KEY FEATURES

The key features of this chapter are the equivalence of Lagrange's equations and **Hamilton's equations**, Hamiltonian **phase space**, **Liouville's theorem** and **recurrence**.

In this chapter we show how Lagrange's equations can be reformulated as a set of *first order* differential equations known as **Hamilton's equations**. Nothing new is added to the physics and the Hamilton formulation is not superior to that of Lagrange when it comes to problem solving. The value of Hamilton's supremely elegant formulation lies in providing a foundation for theoretical extensions both within and outside classical mechanics. Within classical mechanics, it is the basis for most further developments such as the Hamilton-Jacobi theory and chaos. Elsewhere, Hamiltonian mechanics provides the best route to statistical mechanics, and the notion of the Hamiltonian is at the heart of quantum mechanics. As applications of the Hamiltonian formulation, we prove Liouville's theorem and Poincaré's recurrence theorem and explore some of their remarkable consequences.

14.1 SYSTEMS OF FIRST ORDER ODES

The standard form for a system of first order ODEs in the n unknown functions $x_1(t), x_2(t), \ldots, x_n(t)$ is

$$\begin{aligned} \dot{x}_1 &= F_1(x_1, x_2, \ldots, x_n, t), \\ \dot{x}_2 &= F_2(x_1, x_2, \ldots, x_n, t), \\ &\vdots \qquad\qquad \vdots \\ \dot{x}_n &= F_n(x_1, x_2, \ldots, x_n, t), \end{aligned} \tag{14.1}$$

where $F_1, F_2, \ldots, F_n$ are given functions of the variables $x_1, x_2, \ldots, x_n, t$. This can also be written in the compact vector form

$$\dot{\boldsymbol{x}} = \boldsymbol{F}(\boldsymbol{x}, t), \tag{14.2}$$

where $\boldsymbol{x}$ and $\boldsymbol{F}$ are the n-dimensional vectors $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$ and $\boldsymbol{F} = (F_1, F_2, \ldots, F_n)$. If the value of $\boldsymbol{x}$ is given when $t = t_0$, the equations $\dot{\boldsymbol{x}} = \boldsymbol{F}(\boldsymbol{x}, t)$ determine the unknowns $\boldsymbol{x}(t)$ at all subsequent times.

A typical example is the **predator-prey** system of equations

$$\dot{x}_1 = ax_1 - bx_1x_2,$$
$$\dot{x}_2 = bx_1x_2 - cx_2,$$

which govern the population density $x_1(t)$ of the prey and the population density $x_2(t)$ of the predator. In this case, $F_1 = ax_1 - bx_1x_2$, and $F_2 = bx_1x_2 - cx_2$.

Converting higher order equations to first order

Higher order ODEs can always be converted into equivalent systems of first order ODEs. For example, consider the **damped oscillator** equation

$$\ddot{x} + 3\dot{x} + 4x = 0. \tag{14.3}$$

If we introduce the new variable v, defined by $v = \dot{x}$, then the second order equation (14.3) for $x(t)$ can be converted into the pair of first order equations

$$\dot{x} = v$$
$$\dot{v} = -3x - 4v,$$

in the unknowns $\{x(t), v(t)\}$. Since this step is reversible, this pair of first order equations is *equivalent* to the original second order equation (14.3). More generally:

Any system of n second order ODEs in n unknowns can be converted into an equivalent system of $2n$ *first order ODEs in* $2n$ *unknowns.*

Consider, for example, the **orbit equations** for a particle of mass m attracted by the gravitation of a mass M fixed at the origin O. In terms of polar coordinates centred on O, the Lagrangian is

$$L = \tfrac{1}{2}m\left(\dot{r}^2 + r^2\dot{\theta}^2\right) + \frac{mMG}{r}.$$

and the corresponding Lagrange equations are

$$\ddot{r} - r\dot{\theta}^2 = -\frac{MG}{r^2}, \qquad 2r\dot{r}\dot{\theta} + r^2\ddot{\theta} = 0,$$

a pair of second order ODEs in the unknowns $\{r(t), \theta(t)\}$. If we now introduce the new variables v_r and v_θ, defined by

$$v_r = \dot{r}, \qquad v_\theta = \dot{\theta},$$

the *two second order* Lagrange equations can be converted into

$$\dot{r} = v_r, \qquad \dot{v}_r = rv_\theta^2 - MG/r^2,$$
$$\dot{\theta} = v_\theta, \qquad \dot{v}_\theta = -2v_rv_\theta/r,$$

an equivalent system of *four first order* ODEs in the four unknowns $\{r, \theta, v_r, v_\theta\}$.

Hamilton form

In the above examples, we have performed the conversion to first order equations by introducing the **coordinate velocities** as new variables. This is not the only choice however. When transforming a system of Lagrange equations to a first order system, we could instead take the **congugate momenta**, defined by

$$p_j = \frac{\partial L}{\partial \dot{q}_j}, \tag{14.4}$$

as the new variables. This seems quite attractive since the Lagrange equations already have the form

$$\dot{p}_j = \frac{\partial L}{\partial q_j} \qquad (1 \le j \le n).$$

The downside is that the right sides $\partial L/\partial q_j$ are functions of $\boldsymbol{q}$, $\dot{\boldsymbol{q}}$, t, and must be transformed to functions of $\boldsymbol{q}$, $\boldsymbol{p}$, t. This is achieved by inverting the equations (14.4) to express the $\dot{\boldsymbol{q}}$ as functions of $\boldsymbol{q}$, $\boldsymbol{p}$, t.

For the Lagrangian in the orbit problem, the conjugate momenta are

$$p_r = \frac{\partial L}{\partial \dot{r}} = m\dot{r}, \qquad p_\theta = \frac{\partial L}{\partial \dot{\theta}} = mr^2\dot{\theta},$$

and these equations are easily inverted* to give

$$\dot{r} = \frac{p_r}{m}, \qquad \dot{\theta} = \frac{p_\theta}{mr^2}.$$

The *two second order* Lagrange equations for the orbit problem are therefore equivalent to the system of *four first order* ODEs

$$\dot{r} = \frac{p_r}{m}, \qquad \dot{p}_r = \frac{p_\theta^2}{mr^3} - \frac{mMG}{r^2},$$

$$\dot{\theta} = \frac{p_\theta}{mr^2}, \qquad \dot{p}_\theta = 0,$$

in the four unknowns $\{r, \theta, p_r, p_\theta\}$. This is the **Hamilton form** of Lagrange's equations for the orbit problem.

Why bother?

The reader is probably wondering what is the point of converting Lagrange's equations into a system of first order ODEs. For the purpose of finding solutions to particular problems, like the orbit problem above, there is no point. Indeed, the new system of first order

* This step is difficult in the general case where there are *n coupled* linear equations to solve for $\dot{q}_1, \ldots, \dot{q}_n$.

equations may be harder to solve than the original second order equations. The real interest lies in the structure of the general theory. When Lagrange's equations are expressed in Hamilton form* *in a general manner*, the result is a system of first order equations of great simplicity and elegance, now known as **Hamilton's equations**. These equations are the foundation of further developments in analytical mechanics, such as the Hamilton-Jacobi theory and chaos. Also, the **Hamiltonian function**, which appears in Hamilton's equations, is at the heart of quantum mechanics.

14.2 LEGENDRE TRANSFORMS

The general problem of converting Lagrange's equations into Hamilton form hinges on the inversion of the equations that define $\boldsymbol{p}$, namely,

$$p_j = \frac{\partial}{\partial \dot{q}_j} L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) \qquad (1 \leq j \leq n), \tag{14.5}$$

so as to express $\dot{\boldsymbol{q}}$ in terms of $\boldsymbol{q}$, $\boldsymbol{p}$, t. This inversion is made easier by the fact that the $\{p_j\}$ are not general functions of $\boldsymbol{q}$, $\dot{\boldsymbol{q}}$ and t, but are the *first partial derivatives of a scalar function*, the Lagrangian $L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)$. It is a remarkable consequence that the inverse formulae can be written in a similar way.† The details of the argument follow below and the results are summarised at the end of the section.

The two-variable case

We develop the transformation theory for the case of functions of two variables. This has all the important features of the general case but is much easier to follow. Suppose that v_1 and v_2 are defined as functions of the variables u_1 and u_2 by the formulae

$$v_1 = \frac{\partial F}{\partial u_1}, \qquad v_2 = \frac{\partial F}{\partial u_2}, \tag{14.6}$$

where $F(u_1, u_2)$ is a given function of u_1 and u_2. Is it possible to write the inverse formulae‡ in the form

$$u_1 = \frac{\partial G}{\partial v_1}, \qquad u_2 = \frac{\partial G}{\partial v_2}, \tag{14.7}$$

---

* This is the form in which the new variables are the conjugate momenta $p_1, \ldots, p_n$. The form in which the new variables are the generalised velocities $\dot{q}_1, \ldots, \dot{q}_n$ does not lead to an elegant theory, and is therefore not used. It is often claimed that it is not *possible* to take the generalised velocities as new variables because 'they are the time derivatives of the generalised coordinates and therefore cannot be independent variables'. This objection is baseless, as the previous examples show. Indeed, if this objection had any substance, the conjugate momenta would be disqualified as well!

† There is a neat way of seeing that this must be true, which may appeal to mathematicians. If $\boldsymbol{v} = \mathrm{grad}_{\boldsymbol{u}} F(\boldsymbol{u})$, then the Jacobian matrix of the transformation from $\boldsymbol{u}$ to $\boldsymbol{v}$ is symmetric. It follows that the Jacobian matrix of the inverse tranformation must also be symmetric, which is precisely the condition that the inverse transformation has the form $\boldsymbol{u} = \mathrm{grad}_{\boldsymbol{v}} G(\boldsymbol{v})$.

‡ We will always suppose that the inverse transformation does exist.

for some function $G(v_1, v_2)$? In the simplest cases one can answer the question by grinding through the details directly. For example, suppose $F = 2u_1^2 + 3u_1u_2 + u_2^2$. Then

$$v_1 = 4u_1 + 3u_2,$$
$$v_2 = 3u_1 + 2u_2.$$

The inverse formulae are easily obtained by solving these equations for u_1, u_2, which gives

$$u_1 = -2v_1 + 3v_2,$$
$$u_2 = 3v_1 - 4v_2.$$

There is no prior reason to expect that these formulae for u_1, u_2 can be expressed in terms of a single function $G(v_1, v_2)$ in the form (14.7), but it *is* true because the right sides of these equations happen to satisfy the necessary **consistency condition**.* Simple integration then shows that (to within a constant)

$$G = -v_1^2 + 3v_1v_2 - 2v_2^2.$$

This result is not a coincidence. Let $F(u_1, u_2)$ now be *any* function of the variables u_1, u_2, and suppose that a function $G(v_1, v_2)$ satisfying equation (14.7) *does* exist. Consider the expression

$$X = F(u_1, u_2) + G(v_1, v_2) - (u_1v_1 + u_2v_2),$$

which, as it stands, is a function of the four independent variables u_1, u_2, v_1, v_2. Suppose now that, in this formula, we imagine† that v_1 and v_2 are replaced by their expressions in terms of u_1 and u_2. Then X becomes a function of the variables u_1 and u_2 only. Its partial derivative with respect to u_1, holding u_2 constant, is then given by

$$\begin{aligned}\frac{\partial X}{\partial u_1} &= \frac{\partial F}{\partial u_1} + \left(\frac{\partial G}{\partial v_1} \times \frac{\partial v_1}{\partial u_1} + \frac{\partial G}{\partial v_2} \times \frac{\partial v_2}{\partial u_1}\right) - \left(v_1 + u_1\frac{\partial v_1}{\partial u_1} + u_2\frac{\partial v_2}{\partial u_1}\right) \\ &= \left(\frac{\partial F}{\partial u_1} - v_1\right) + \left(\frac{\partial G}{\partial v_1} - u_1\right)\frac{\partial v_1}{\partial u_1} + \left(\frac{\partial G}{\partial v_2} - u_2\right)\frac{\partial v_2}{\partial u_1} \\ &= 0 + 0 + 0 = 0,\end{aligned}$$

* If $u_1 = f_1(v_1, v_2)$ and $u_2 = f_2(v_1, v_2)$ then it is possible to express u_1, u_2 in the form (14.7) only if the functions f_1 and f_2 are related by the formula

$$\frac{\partial f_1}{\partial v_2} = \frac{\partial f_2}{\partial v_1},$$

which is called the **consistency condition**.

† Pure mathematicians strongly object to such feats of imagination. Unfortunately, the alternative is to introduce a welter of functional notation which obscures the essential simplicity of the argument. We will make frequent use of such 'imagined' substitutions.

on using first the chain rule and then the formulae (14.6) and (14.7). Hence X is independent of the variable u_1. In exactly the same way we may show that $\partial X/\partial u_2 = 0$ so that X is also independent of u_2. It follows that X must be a constant! This constant can be absorbed into the function G without disturbing the formulae (14.7), in which case $X = 0$. We have therefore shown that if F and G are related by the equations (14.6) and (14.7), then they must* satisfy the relation

$$F(u_1, u_2) + G(v_1, v_2) = u_1 v_1 + u_2 v_2. \tag{14.8}$$

The above argument is reversible so the converse result is also true. We have therefore shown that:

The required function $G(v_1, v_2)$ ***always exists*** *and can be generated from the function $F(u_1, u_2)$ by the formula*

$$\boxed{G(v_1, v_2) = (u_1 v_1 + u_2 v_2) - F(u_1, u_2)} \tag{14.9}$$

where u_1 and u_2 are to be replaced by their expressions in terms of v_1 and v_2.

It is evident that the relationship between the functions F and G is a symmetrical one. Each function is said to be the **Legendre transform** of the other.

Example 14.1 *Finding a Legendre transform*

Find the Legendre transform of the function $F(u_1, u_2) = 2u_1^2 + 3u_1u_2 + u_2^2$ by using the formula (14.9).

Solution

For this F, $v_1 = \partial F/\partial u_1 = 4u_1 + 3u_2$ and $v_2 = \partial F/\partial u_2 = 3u_1 + 2u_2$. The inverse formulae are $u_1 = -2v_1 + 3v_2$ and $u_2 = 3v_1 - 4v_2$. From equation (14.9), the function G is given by

$$\begin{aligned} G &= u_1 v_1 + u_2 v_2 - F(u_1, u_2) \\ &= (-2v_1 + 3v_2)v_1 + (3v_1 - 4v_2)v_2 - F(-2v_1 + 3v_2, 3v_1 - 4v_2) \\ &= -2v_1^2 + 6v_1 v_2 - 4v_2^2 - \\ &\quad \Big(2(-2v_1 + 3v_2)^2 + 3(-2v_1 + 3v_2)(3v_1 - 4v_2) + (3v_1 - 4v_2)^2\Big) \\ &= -v_1^2 + 3v_1 v_2 - 2v_2^2, \end{aligned}$$

the same as was obtained directly. This is the **Legendre transform** of the given function F. ■

* As we have seen, this may require a constant to be added to the function G.

Active and passive variables

The variables $\boldsymbol{u} = (u_1, u_2)$ and $\boldsymbol{v} = (v_1, v_2)$ are called **active variables** because they are the ones that are actually transformed. However, the functions F and G may also depend on additional variables that are not part of the transformation as such, but have the status of parameters. These are called **passive variables**. In the dynamical problem, $\dot{\boldsymbol{q}}$ and $\boldsymbol{p}$ are the active variables and $\boldsymbol{q}$ is the passive variable. We need to find how partial derivatives of F and G with respect to the passive variables are related.

Suppose then that $F = F(u_1, u_2, w)$ and $G = G(v_1, v_2, w)$ satisfy the formulae (14.6) and (14.7), where w is a passive variable. Then (14.6) defines v_1, v_2 as functions of u_1, u_2 and w, and (14.7) defines u_1, u_2 as functions of v_1, v_2 and w. The argument leading to the formula (14.8) still holds so that

$$F(u_1, u_2, w) + G(v_1, v_2, w) = u_1 v_1 + u_2 v_2. \tag{14.10}$$

In this formula, imagine that v_1 and v_2 are replaced by their expressions in terms of u_1, u_2 and w; then differentiate the resulting identity with respect to w, holding u_1 and u_2 constant. On using the chain rule, this gives

$$\frac{\partial F}{\partial w} + \left(\frac{\partial G}{\partial v_1} \times \frac{\partial v_1}{\partial w} + \frac{\partial G}{\partial v_2} \times \frac{\partial v_2}{\partial w} + \frac{\partial G}{\partial w} \right) = u_1 \frac{\partial v_1}{\partial w} + u_2 \frac{\partial v_2}{\partial w},$$

which can be written

$$\frac{\partial F}{\partial w} + \frac{\partial G}{\partial w} = \left(u_1 - \frac{\partial G}{\partial v_1} \right) \frac{\partial v_1}{\partial w} + \left(u_2 - \frac{\partial G}{\partial v_2} \right) \frac{\partial v_2}{\partial w} = 0 + 0 = 0,$$

on using the relations (14.7). Hence the partial derivatives of $F(u_1, u_2, w)$ and $G(v_1, v_2, w)$ with respect to w are related by

$$\boxed{\frac{\partial F}{\partial w} = -\frac{\partial G}{\partial w}} \tag{14.11}$$

This is the required result; it holds for *each* passive variable w.

The general case with many variables

The preceding theory can be extended to any number of variables. The results are exactly what one would expect and are summarised in the box below. This summary is presented in a compact vector form using the n-dimensional 'grad'.* It is a good idea to write these results out in expanded form.

* If $F = F(\boldsymbol{u}, \boldsymbol{w})$, where $\boldsymbol{u} = (u_1, u_2, \ldots, u_n)$ and $\boldsymbol{w} = (w_1, w_2, \ldots, w_m)$, then $\operatorname{grad}_{\boldsymbol{u}} F$ and $\operatorname{grad}_{\boldsymbol{w}} F$ mean

$$\operatorname{grad}_{\boldsymbol{u}} F(\boldsymbol{u}, \boldsymbol{w}) = \left(\frac{\partial F}{\partial u_1}, \frac{\partial F}{\partial u_2}, \cdots, \frac{\partial F}{\partial u_n} \right), \qquad \operatorname{grad}_{\boldsymbol{w}} F(\boldsymbol{u}, \boldsymbol{w}) = \left(\frac{\partial F}{\partial w_1}, \frac{\partial F}{\partial w_2}, \cdots, \frac{\partial F}{\partial w_m} \right).$$

Legendre transforms

Suppose that the variables $\boldsymbol{v} = (v_1, v_2, \ldots, v_n)$ are defined as functions of the active variables $\boldsymbol{u} = (u_1, u_2, \ldots, u_n)$ and passive variables $\boldsymbol{w} = (w_1, w_2, \ldots, w_m)$ by the formula

$$\boldsymbol{v} = \operatorname{grad}_{\boldsymbol{u}} F(\boldsymbol{u}, \boldsymbol{w}), \tag{14.12}$$

where F is a given function of $\boldsymbol{u}$ and $\boldsymbol{w}$. Then the inverse formula can always be written in the form

$$\boldsymbol{u} = \operatorname{grad}_{\boldsymbol{v}} G(\boldsymbol{v}, \boldsymbol{w}), \tag{14.13}$$

where the function $G(\boldsymbol{v}, \boldsymbol{w})$ is related to the function $F(\boldsymbol{u}, \boldsymbol{w})$ by the formula

$$G(\boldsymbol{v}, \boldsymbol{w}) = \boldsymbol{u} \cdot \boldsymbol{v} - F(\boldsymbol{u}, \boldsymbol{w}), \tag{14.14}$$

where $\boldsymbol{u} \cdot \boldsymbol{v} = u_1 v_1 + u_2 v_2 + \cdots + u_n v_n$.

Furthermore, the derivatives of F and G with respect to the passive variables $\{w_j\}$ are related by

$$\operatorname{grad}_{\boldsymbol{w}} F(\boldsymbol{u}, \boldsymbol{w}) = -\operatorname{grad}_{\boldsymbol{w}} G(\boldsymbol{v}, \boldsymbol{w}). \tag{14.15}$$

The relationship between the functions F and G is symmetrical and each is said to be the **Legendre transform** of the other.

14.3 HAMILTON'S EQUATIONS

Let $\mathcal{S}$ be a Lagrangian mechanical system with n degrees of freedom and generalised **coordinates** $\boldsymbol{q} = (q_1, q_1, \ldots, q_n)$. Then the Lagrange equations of motion for $\mathcal{S}$ are

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \frac{\partial L}{\partial q_j} = 0 \qquad (1 \leq j \leq n), \tag{14.16}$$

where $L = L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)$ is the Lagrangian of $\mathcal{S}$. This is a set of n second order ODEs in the unknowns $\boldsymbol{q}(t) = (q_1(t), q_2(t), \ldots, q_n(t))$. We now wish to convert these equations into **Hamilton form**, that is, an equivalent set of $2n$ first order ODEs in the $2n$ unknowns $\boldsymbol{q}(t)$, $\boldsymbol{p}(t)$, where $\boldsymbol{p}(t) = (p_1(t), p_2(t), \ldots, p_n(t))$, where the $\{p_j\}$ are the generalised **momenta** of $\mathcal{S}$. The $\{p_j\}$ are defined by

$$p_j = \frac{\partial L}{\partial \dot{q}_j} \qquad (1 \leq j \leq n), \tag{14.17}$$

which can be written in the vector form

$$\boldsymbol{p} = \operatorname{grad}_{\dot{\boldsymbol{q}}} L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t). \tag{14.18}$$

The first step is to eliminate the coordinate velocities $\dot{\boldsymbol{q}}$ from the Lagrange equations in favour of the momenta $\boldsymbol{p}$. This in turn requires that the formula (14.18) must be inverted so as to express $\dot{\boldsymbol{q}}$ in terms of $\boldsymbol{q}$, $\boldsymbol{p}$ and t. *This is precisely what Legendre transforms do*. It follows from the theory of the last section that the inverse formula to (14.18) can be written in the form

$$\dot{\boldsymbol{q}} = \operatorname{grad}_{\boldsymbol{p}} H(\boldsymbol{q}, \boldsymbol{p}, t), \tag{14.19}$$

where the function $H(\boldsymbol{q}, \boldsymbol{p}, t)$ is the **Legendre transform** of the Lagrangian function $L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)$. Here, $\dot{\boldsymbol{q}}$ and $\boldsymbol{p}$ are the active variables and $\boldsymbol{q}$ is the passive variable.

Definition 14.1 ***Hamiltonian function*** *The function $H(\boldsymbol{q}, \boldsymbol{p}, t)$, which is the Legendre transform of the Lagrangian function $L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)$, is called the* ***Hamiltonian function*** *of the system $\mathcal{S}$.*

Since the functions H and L are Legendre transforms of each other, they satisfy the relations

$$\boxed{H(\boldsymbol{q}, \boldsymbol{p}, t) = \dot{\boldsymbol{q}} \cdot \boldsymbol{p} - L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)} \tag{14.20}$$

which can be used to generate H from L, and

$$\operatorname{grad}_{\boldsymbol{q}} L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) = -\operatorname{grad}_{\boldsymbol{q}} H(\boldsymbol{q}, \boldsymbol{p}, t), \tag{14.21}$$

which connects the derivatives of L and H with respect to the passive variables.

It is now quite easy to perform the transformation of Lagrange's equations. The Lagrange equations (14.16) can be written in terms of the generalised momenta $\{p_j\}$ in the form

$$\dot{p}_j = \frac{\partial L}{\partial q_j} \qquad (1 \leq j \leq n),$$

which is equivalent to the vector form

$$\dot{\boldsymbol{p}} = \operatorname{grad}_{\boldsymbol{q}} L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t). \tag{14.22}$$

The right sides of these equations still involve $\dot{\boldsymbol{q}}$, but, on using the formula (14.21), we obtain

$$\dot{\boldsymbol{p}} = -\operatorname{grad}_{\boldsymbol{q}} H(\boldsymbol{q}, \boldsymbol{p}, t). \tag{14.23}$$

These are the transformed Lagrange equations! *The* ***Hamilton form*** *of the Lagrange equations therefore consists of equations (14.23) together with equations (14.19), which effectively define the generalised momentum $\boldsymbol{p}$.*

All of the above argument is reversible and so the Hamilton form and the Lagrange form are equivalent. Our results are summarised below:

Hamilton's equations

The n Lagrange equations (14.16) are equivalent to the system of $2n$ first order ODEs

$$\dot{\boldsymbol{q}} = \operatorname{grad}_{\boldsymbol{p}} H(\boldsymbol{q}, \boldsymbol{p}, t), \qquad \dot{\boldsymbol{p}} = -\operatorname{grad}_{\boldsymbol{q}} H(\boldsymbol{q}, \boldsymbol{p}, t), \tag{14.24}$$

where the **Hamiltonian function** $H(\boldsymbol{q}, \boldsymbol{p}, t)$ is the Legendre transform of the Lagrangian $L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)$ and is generated by the formula (14.20). This is the vector form of **Hamilton's equations**.* The expanded form is

$$\dot{q_j} = \frac{\partial H}{\partial p_j}, \qquad \dot{p_j} = -\frac{\partial H}{\partial q_j} \qquad (1 \leq j \leq n).$$

We have shownthat the n second order Lagrange equations in the n unknowns $\boldsymbol{q}(t)$ are mathematically equivalent to the $2n$ first order Hamilton equations in the $2n$ unknowns $\boldsymbol{q}(t)$, $\boldsymbol{p}(t)$. In each of these formulations of mechanics, the motion of the system is determined by the form of a single function, the **Lagrangian** $L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)$ in the Lagrange formulation, and the **Hamiltonian** $H(\boldsymbol{q}, \boldsymbol{p}, t)$ in the Hamilton formulation. Hamilton's equations are a particularly elegant first order system in which the functions $F_1, F_2, \ldots$ that appear on the right are simply the first partial derivatives of a *single* function, the Hamiltonian H. Moreover these right hand sides also satisfy the special condition† $\operatorname{div} \boldsymbol{F} = 0$, which allows Liouville's theorem to be applied to Hamiltonian mechanics.‡

Explicit time dependence

One final note. When the Lagrangian has an *explicit* time dependence, this t has the status of an extra passive variable. It follows that we then have the additional relation

$$\frac{\partial L}{\partial t} = -\frac{\partial H}{\partial t}, \tag{14.25}$$

* After Sir William Rowan Hamilton, whose paper *Second Essay on a General Method in Dynamics* was published in 1835. Hamilton's equations are sometimes called the *canonical equations*; no one seems to know the reason why.

† The scalar quantity $\operatorname{div} \boldsymbol{F}$ is defined by

$$\operatorname{div} \boldsymbol{F} = \frac{\partial F_1}{\partial x_1} + \frac{\partial F_2}{\partial x_2} + \cdots + \frac{\partial F_n}{\partial x_n}.$$

‡ None of these statements is true if Lagrange's equations are expressed as a first order system by taking the coordinate *velocities* $\dot{\boldsymbol{q}}$ as the new variables.

which shows that if either of L or H has an explicit time dependence, then so does the other.

Example 14.2 *Finding a Hamiltonian and Hamilton's equations*

Find the Hamiltonian and Hamilton's equations for the simple pendulum.

Solution

The **Lagrangian** for the simple pendulum is

$$L = \tfrac{1}{2}ma^2\dot{\theta}^2 + mga\cos\theta,$$

where θ is the angle between the string and the downward vertical, m is the mass of the bob, and a is the string length. The momentum p_θ conjugate to the coordinate θ is given by

$$p_\theta = \frac{\partial L}{\partial \dot{\theta}} = ma^2\dot{\theta}$$

and this formula is easily inverted to give

$$\dot{\theta} = \frac{p_\theta}{ma^2}. \tag{14.26}$$

The Hamiltonian H is then given by

$$H = \dot{\theta}\, p_\theta - L,$$

where $\dot{\theta}$ is given by equation (14.26). This gives

$$\begin{aligned} H &= \left(\frac{p_\theta}{ma^2}\right) p_\theta - \tfrac{1}{2}ma^2\left(\frac{p_\theta}{ma^2}\right)^2 - mga\cos\theta \\ &= \frac{p_\theta^2}{2ma^2} - mga\cos\theta. \end{aligned}$$

This is the **Hamiltonian** for the simple pendulum. From H we can find Hamilton's equations. They are

$$\begin{aligned} \dot{\theta} &= \frac{\partial H}{\partial p_\theta} = \frac{p_\theta}{ma^2}, \\ \dot{p_\theta} &= -\frac{\partial H}{\partial \dot{\theta}} = -mga\sin\theta. \end{aligned}$$

These are **Hamilton's equations** for the simple pendulum.

This simple example illustrates clearly why Lagrange's equations are preferred over Hamilton's equations for the *practical* solution of problems. To solve Hamilton's equations in this case, we would differentiate the first equation with respect to t and then use the second equation to eliminate the unknown p_θ. This gives

$$\ddot{\theta} + \frac{g}{a}\sin\theta = 0,$$

which is precisely the Lagrange equation for the system! ■

Properties of the Hamiltonian H

The Hamiltonian function $H(\boldsymbol{q}, \boldsymbol{p}, t)$ has been defined as the Legendre transform of $L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)$ and, as such, it can be generated by the formula (14.20). We have met this expression before. It is identical to the **energy function** h

$$h = \sum_{j=1}^{n} \dot{q}_j p_j - L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t), \tag{14.27}$$

defined in section 12.8. The only difference between h and H is that the functional form of H is vital. H *must* be be expressed in terms of the variables $\boldsymbol{q}$, $\boldsymbol{p}$, t. On the other hand, since only the *values* taken by h are significant, its functional form is unimportant and it may be expressed in terms of any variables. However, since the values taken by H and h are the same, the results that we obtained in section 12.8 concerning h must also be true for the Hamiltonian H. In particular, when H has **no explicit time dependence**, H is a **constant of the motion**.* This result can also be proved independently, as follows.

Suppose that $H = H(\boldsymbol{q}, \boldsymbol{p})$ and that $\{\boldsymbol{q}(t), \boldsymbol{p}(t)\}$ is a motion of the system. Then, in this motion,

$$\begin{aligned}\frac{dH}{dt} &= \sum_{j=1}^{n} \frac{\partial H}{\partial q_j}\dot{q}_j + \sum_{j=1}^{n} \frac{\partial H}{\partial p_j}\dot{p}_j \\ &= \sum_{j=1}^{n} \frac{\partial H}{\partial q_j}\left(\frac{\partial H}{\partial p_j}\right) + \sum_{j=1}^{n} \frac{\partial H}{\partial p_j}\left(-\frac{\partial H}{\partial q_j}\right) \\ &= 0,\end{aligned}$$

where the first step follows from the chain rule and the second from Hamilton's equations. Hence H remains constant in the motion.

Systems for which $H = H(\boldsymbol{q}, \boldsymbol{p})$ are said to be **autonomous**. (This term was previously applied to systems for which $L = L(\boldsymbol{q}, \dot{\boldsymbol{q}})$, but equation (14.25) shows that these two classes of systems are the same.) The above result can therefore be expressed in the form:

Autonomous systems conserve H

In any motion of an autonomous system, the Hamiltonian $H(\boldsymbol{q}, \boldsymbol{p})$ is conserved.

In addition, when $\mathcal{S}$ is a **conservative standard system**, the Hamiltonian H can be expressed in the simpler form

$$H(\boldsymbol{q}, \boldsymbol{p}) = T(\boldsymbol{q}, \boldsymbol{p}) + V(\boldsymbol{q}) \tag{14.28}$$

* As we remarked earlier, H has an explicit time dependence when L does; the circumstances under which this occurs are listed in section 12.6.

where $T(\boldsymbol{q}, \boldsymbol{p})$ is the kinetic energy of the system expressed in terms of the variables $\boldsymbol{q}, \boldsymbol{p}$. *In this case, H is simply the* ***total energy*** *of the system, expressed in terms of the variables $\boldsymbol{q}, \boldsymbol{p}$.* This is the quickest way of finding H when the system is conservative.

Example 14.3 *Finding a Hamiltonian 2*

Find the Hamiltonian for the inverse square orbit problem considered earlier and deduce Hamilton's equations for this system.

Solution

This is a **conservative** system so that $H = T + V$. With the polar coordinates r and θ as generalised coordinates, T and V are given by

$$T = \tfrac{1}{2}m\left(\dot{r}^2 + r^2\dot{\theta}^2\right) \qquad V = -\frac{mMG}{r}.$$

and the generalised momenta are given by

$$p_r = \frac{\partial L}{\partial \dot{r}} = m\dot{r}, \qquad p_\theta = \frac{\partial L}{\partial \dot{\theta}} = mr^2\dot{\theta}.$$

These equations are easily inverted to give

$$\dot{r} = \frac{p_r}{m}, \qquad \dot{\theta} = \frac{p_\theta}{mr^2}$$

so that the Hamiltonian is given by

$$\begin{aligned} H = T + V &= \tfrac{1}{2}m\left(\dot{r}^2 + r^2\dot{\theta}^2\right) - \frac{mMG}{r} \\ &= \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} - \frac{mMG}{r}. \end{aligned}$$

This is the required **Hamiltonian**. Hamilton's equations are now found by using this Hamiltonian in the general equations (14.25). The partial derivatives of H are

$$\frac{\partial H}{\partial p_r} = \frac{p_r}{m}, \qquad \frac{\partial H}{\partial p_\theta} = \frac{p_\theta}{mr^2}, \qquad \frac{\partial H}{\partial r} = -\frac{p_\theta^2}{mr^3}, \qquad \frac{\partial H}{\partial \theta} = 0$$

and **Hamilton's equations** for the orbit problem are therefore

$$\dot{r} = \frac{p_r}{m}, \qquad \dot{p}_r = \frac{p_\theta^2}{mr^3} - \frac{mMG}{r^2},$$

$$\dot{\theta} = \frac{p_\theta}{mr^2}, \qquad \dot{p}_\theta = 0.$$

Naturally, these are the same equations as were obtained earlier by 'manual' transformation of Lagrange's equations. As in the last example, solution of the Hamilton equations by eliminating the momenta simply leads back to Lagrange's equations. ■

Momentum conservation

From the Hamilton equation $\dot{p}_j = -\partial H/\partial q_j$, it follows that:

If $\partial H/\partial q_j = 0$ (that is, if the coordinate q_j is absent from the Hamiltonian), then the generalised momentum p_j is constant in any motion.

The corresponding result in the Lagrangian formulation is that:

If $\partial L/\partial q_j = 0$ (that is, if the coordinate q_j is absent from the Lagrangian), then the generalised momentum p_j is constant in any motion.

These two results seem slightly different, but they *are* equivalent, since, from equation (14.21), $\partial H/\partial q_j = -\partial L/\partial q_j$. This means that the term **cyclic coordinate**, by which we previously meant a coordinate that did not appear in the *Lagrangian*, can be applied without ambiguity to mean that the coordinate does not appear in the *Hamiltonian*. Our result is then:

Conservation of momentum

If q_j is a cyclic coordinate (in the sense that it does not appear in the Hamiltonian), then p_j, the generalised momentum conjugate to q_j, is constant in any motion.

14.4 HAMILTONIAN PHASE SPACE ($(\boldsymbol{q}, \boldsymbol{p})$–space)

Suppose the mechanical system $\mathcal{S}$ has generalised coordinates $\boldsymbol{q}$, conjugate momenta $\boldsymbol{p}$, and Hamiltonian $H(\boldsymbol{q}, \boldsymbol{p}, t)$. If the initial values of $\boldsymbol{q}$ and $\boldsymbol{p}$ are known,* then the subsequent motion of $\mathcal{S}$, described by the functions $\{\boldsymbol{q}(t), \boldsymbol{p}(t)\}$, is uniquely determined by Hamilton's equations. This motion can be represented geometrically by the motion of a 'point' (called a **phase point**) in Hamiltonian **phase space**. Hamiltonian phase space is a real space of $2n$ dimensions in which a 'point' is a set of values $(q_1, q_2, \ldots, q_n, p_1, p_2, \ldots, p_n)$ of the independent variables $\{\boldsymbol{q}, \boldsymbol{p}\}$. (Note that a point in Hamiltonian phase space represents not only the configuration of the system $\mathcal{S}$ but also its instantaneous momenta. This is the distinction between Hamiltonian phase space, which has $2n$ dimensions, and Lagrangian configuration space, which has n dimensions.) Each motion of the system $\mathcal{S}$ then corresponds to the motion of a phase point through the phase space.†

The only case in which we can actually draw the phase space is when $\mathcal{S}$ has just one degree of freedom. Then the phase space is two-dimensional and can be drawn on paper.

---

* We are more familiar with initial conditions in which $\boldsymbol{q}$ and $\dot{\boldsymbol{q}}$ are prescribed. However, these conditions are equivalent to those in which the initial values of $\boldsymbol{q}$ and $\boldsymbol{p}$ are prescribed.

† It should be noted that *Hamiltonian* phase space is generally not the same as the phase space introduced in Chapter 8, which, in the present notation, is $(\boldsymbol{q}, \dot{\boldsymbol{q}})$-space. In particular, our next result (Liouville's theorem) does not apply in $(\boldsymbol{q}, \dot{\boldsymbol{q}})$-space.

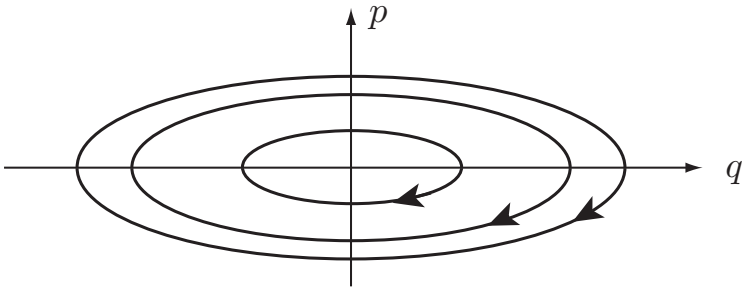

FIGURE 14.1 Typical paths in the phase space (q, p) corresponding to motions of a system $\mathcal{S}$ with Hamiltonian $H = p^2 + q^2/9$. The arrows show the direction that the phase point moves along each path as t increases.

Example 14.4 *Paths in phase space*

Suppose that $\mathcal{S}$ has the single coordinate q and Lagrangian

$$L = \frac{\dot{q}^2}{4} - \frac{q^2}{9}.$$

Find the paths in Hamiltonian phase space that correspond to the motions of $\mathcal{S}$.

Solution

The conjugate momentum $p = \partial L/\partial \dot{q} = \frac{1}{2}\dot{q}$, and the Hamiltonian is

$$H = \dot{q}\,p - L = (2p)\,p - \frac{1}{4}\,(2p)^2 + \frac{q^2}{9} = p^2 + \frac{q^2}{9}.$$

Hamilton's equations for $\mathcal{S}$ are therefore

$$\dot{q} = 2p, \qquad \dot{p} = -2q/9.$$

On eliminating p, we find that q satisfies the SHM equation

$$\ddot{q} + (4q/9) = 0.$$

The general solution of the Hamilton equations for $\mathcal{S}$ is therefore

$$q = 3A\cos((2t/3) + \alpha), \qquad p = -A\sin((2t/3) + \alpha),$$

where A and α are arbitrary constants. These are the parametric equations of the **paths** in phase space, the parameter being the time t; each path corresponds to a possible motion of the system $\mathcal{S}$. Some typical paths are shown in Figure 14.1. For this system , every motion is periodic so that the paths are *closed* curves in the (q, p)-plane. (They are actually concentric similar ellipes.) The arrows show the direction that the phase point moves along each path as t increases. ■

Of course, most mechanical systems have more than one degree of freedom so that the corresponding phase space has dimension four or more and cannot be drawn. If the system consists of a mole of gas molecules, the dimension of the phase space is six times Avogadro's number! Nevertheless, the notion of phase space is still valuable for we can still apply **geometrical reasoning** to spaces of higher dimension. This will not *solve* Hamilton's equations of motion, but it does enable us to make valuable predictions about the nature of the motion.

The phase fluid

The paths of phase points have a simpler structure when the system is **autonomous**, that is, $H = H(\boldsymbol{q}, \boldsymbol{p})$. In this case, H is a constant of the motion, so that each phase path must lie on a 'surface'* of constant energy† within the phase space. Thus the phase space is filled with the non-intersecting level surfaces of H, like layers in a multi-dimensional onion, and each phase path is restricted to one of these level surfaces.

For autonomous systems, *there can only be one phase path passing through any point of the phase space*. The reason is as follows: suppose that one phase point is at the point $(\boldsymbol{q}_0, \boldsymbol{p}_0)$ at time t_1, and another phase point is at $(\boldsymbol{q}_0, \boldsymbol{p}_0)$ at time t_2. Then, since H is independent of t, the second motion can be obtained from the first by simply making the substitution $t \to t + t_1 - t_2$, a shift in the origin of time. Therefore the two phase points travel along the *same path* with the second point delayed relative to the first by the constant time $t_2 - t_1$. Hence **phase paths cannot intersect**. This means that the phase space is filled with non-intersecting phase paths like the **streamlines** of a fluid in steady flow. Each motion of the system $\mathcal{S}$ corresponds to a phase point moving along one of these paths, just as the real particles of a fluid move along the fluid streamlines. The $2n$-dimensional vector quantity $\boldsymbol{u} = (\dot{\boldsymbol{q}}, \dot{\boldsymbol{p}})$ has the rôle of the fluid velocity field $\boldsymbol{u}(\boldsymbol{r})$‡ and Hamilton's equations serve to specify what this velocity is at the point $(\boldsymbol{q}, \boldsymbol{p})$ of the phase space. Because of this analogy with fluid mechanics, the motion of phase points in phase space is called the **phase flow**.

14.5 LIOUVILLE'S THEOREM AND RECURRENCE

Consider those phase points that, at some instant, occupy the region $\mathcal{R}_0$ of the phase space, as shown in Figure 14.2. As t increases, these points move along their various phase paths in accordance with Hamilton's equations and, after time t, will occupy some new region $\mathcal{R}_t$ of the phase space. This new region will have a different shape§

* If the phase space has dimension six, then a 'surface' of constant H has dimension five. This is therefore a generalisation of the notion of surface, which normally has dimension two.

† This 'energy' is the generalised energy $H(\boldsymbol{q}, \boldsymbol{p})$. For a conservative system, it is equal to the actual total energy $T + V$.

‡ $\boldsymbol{u}(\boldsymbol{r})$ is the velocity of the fluid particle instantaneously at the point with position vector $\boldsymbol{r}$.

§ Since the motion of many systems is sensitive to the initial conditions, the shape of $\mathcal{R}_t$ can become very weird indeed!

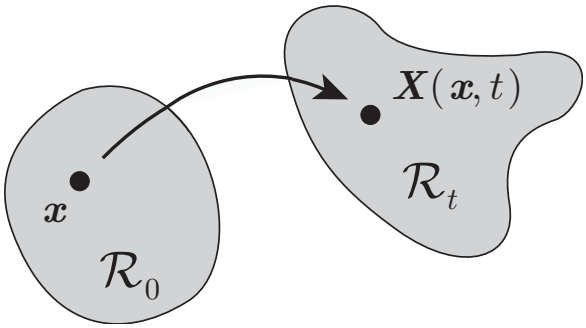

FIGURE 14.2 Liouville's theorem: the Hamiltonian phase flow preserves volume.

to $\mathcal{R}_0$, but **Liouville's theorem*** states that the volumes† of the two regions are equal. This remarkable result is expressed by saying that the *Hamiltonian phase flow preserves volume*. The theorem is easy to apply, but the proof is rather difficult.

Proof of Liouville's theorem

The proof is easier to follow if we use $x_1, x_2, \ldots, x_{2n}$ as the names of the variables (instead of $\boldsymbol{q}$, $\boldsymbol{p}$), and also call the right sides of Hamilton's equations $F_1, F_2, \ldots, F_{2n}$. Then, in vector notation, the equations of motion are $\dot{\boldsymbol{x}} = \boldsymbol{F}(\boldsymbol{x}, t)$. We will give the details for the case when the phase space is two-dimensional; the method in the general case is the same but uglier.

Consider a set of phase points moving in the (x_1, x_2)-plane, which, at some instant in time, occupies the region $\mathcal{R}_0$, as shown in Figure 14.2. Without losing generality, we may suppose that this occurs at time $t = 0$. After time t, a typical point $\boldsymbol{x}$ of $\mathcal{R}_0$ has moved on to position $\boldsymbol{X} = \boldsymbol{X}(\boldsymbol{x}, t)$ and the set as a whole now occupies the region $\mathcal{R}_t$. In this two-dimensional case, the 'volume' $v(t)$ of $\mathcal{R}_t$ is the *area* of this region in the (x_1, x_2)-plane. Now

$$v(t) = \int_{\mathcal{R}_t} dX_1 dX_2 = \int_{\mathcal{R}_0} J\, dx_1 dx_2,$$

where J is the Jacobian of the transformation $\boldsymbol{X} = \boldsymbol{X}(\boldsymbol{x}, t)$, that is,

$$J = \begin{vmatrix} \partial X_1/\partial x_1 & \partial X_1/\partial x_2 \\ \partial X_2/\partial x_1 & \partial X_2/\partial x_2 \end{vmatrix}. \tag{14.29}$$

Now, for small t, $\boldsymbol{X}$ may be approximated by

$$\begin{aligned} \boldsymbol{X}(\boldsymbol{x}, t) &= \boldsymbol{X}(\boldsymbol{x}, 0) + t\, \frac{\partial \boldsymbol{X}}{\partial t}(\boldsymbol{x}, 0) + O(t^2) \\ &= \boldsymbol{x} + t\, \boldsymbol{F}(\boldsymbol{x}, 0) + O(t^2), \end{aligned}$$

on using the equation of motion $\dot{\boldsymbol{x}} = \boldsymbol{F}(\boldsymbol{x}, t)$. The corresponding approximation for J is

$$J = 1 + t \left[\frac{\partial F_1}{\partial x_1} + \frac{\partial F_2}{\partial x_2} \right]_{t=0} + O(t^2) = 1 + t\, \mathrm{div}\, \boldsymbol{F}(\boldsymbol{x}, 0) + O(t^2).$$

* After the French mathematician Joseph Liouville (1809–1882).

† Since the dimension of the phase space can be any (even) number, this is a generalisation of the notion of volume.

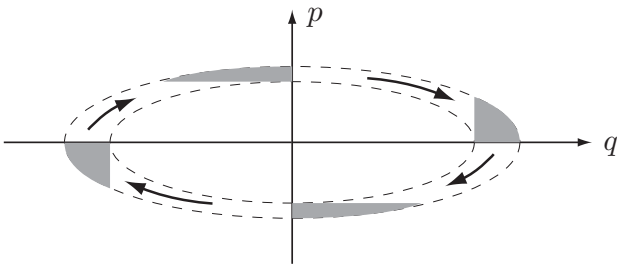

FIGURE 14.3 An instance of Liouville's theorem with the Hamiltonian $H = p^2 + q^2/9$. The shaded region moves through the phase space. Its shape changes but its area remains the same.

Hence the volume of $\mathcal{R}_t$ is approximated by

$$v(t) = \int_{\mathcal{R}_0} \Big(1 + t \operatorname{div} \boldsymbol{F}(\boldsymbol{x}, 0)\Big)\, dx_1 dx_2 + O(t^2)$$

when t is small. It follows that

$$\left.\frac{dv}{dt}\right|_{t=0} = \lim_{t\to 0}\left(\frac{v(t) - v(0)}{t}\right) = \int_{\mathcal{R}_0} \operatorname{div} \boldsymbol{F}(\boldsymbol{x}, 0)\; dx_1 dx_2.$$

Finally, since the initial instant $t = 0$ was arbitrarily chosen, this result must apply for any t, that is,

$$\frac{dv}{dt} = \int_{\mathcal{R}_t} \operatorname{div} \boldsymbol{F}(\boldsymbol{x}, t)\; dx_1 dx_2$$

at any time t. We see that, for *general* systems of equations, the phase flow does *not* preserve volume. However, if $\operatorname{div} \boldsymbol{F}(\boldsymbol{x}, t) = 0$, then volume *is* preserved. For the case of Hamilton's equations with one degree of freedom,

$$\begin{aligned}\operatorname{div} \boldsymbol{F} &= \frac{\partial F_1}{\partial x_1} + \frac{\partial F_2}{\partial x_2} \\ &= \frac{\partial}{\partial q}\left(\frac{\partial H}{\partial p}\right) + \frac{\partial}{\partial p}\left(-\frac{\partial H}{\partial q}\right) = 0.\end{aligned}$$

Hence the Hamiltonian phase flow satisfies the condition $\operatorname{div} \boldsymbol{F} = 0$ and so preserves volume. This completes the proof. ■

Liouville's theorem

The motions of a Hamiltonian system preserve volume in $(\boldsymbol{q}, \boldsymbol{p})$-space.

A particular instance of Liouville's theorem is shown in Figure 14.3. The phase paths of the Hamiltonian $H = p^2 + q^2/9$, shown in Figure 14.1, are concentric similar ellipses. Figure 14.3 shows the progress of a region of the phase space lying between two such elliptical paths. The region changes shape but its area remains the same.

Liouville's theorem has many applications and is particularly important in statistical mechanics. The following is a simple example.

Example 14.5 ***No limit cycles in Hamiltonian mechanics***

In the theory of dynamical systems, a periodic solution is said to be an *asymptotically stable limit cycle* if it 'attracts' points in nearby volumes of the phase space (see Chapter 8). Show that limit cycles cannot occur in the dynamics of Hamiltonian systems.

Solution

Suppose there were a closed path $\mathcal{C}$ in the phase space that attracts points in a nearby region $\mathcal{R}$. Then eventually the points that lay in $\mathcal{R}$ must lie in a narrow 'tube' of *arbitrarily small* 'radius' enclosing the path $\mathcal{C}$. The volume of this tube tends to zero with increasing time so that the original volume of $\mathcal{R}$ cannot be be preserved. This is contrary to Liouville's theorem and so asymptotically stable limit cycles cannot exist. ■

Poincaré's theorem and recurrence

Many Hamiltonian systems have the property that each path is confined to some **bounded region** within the phase space. Typically this is a consequence of **energy conservation**, where the energy surfaces happen to be bounded. Liouville's theorem has startling implications concerning the motion of such systems. First, we need to prove a result known as **Poincaré's recurrence theorem**. Poincaré's theorem is actually a result from ergodic theory and has many applications outside classical mechanics. However, since we are going to apply it to phase space, we will prove it in that context.

Theorem 14.1 ***Poincaré's recurrence theorem*** *Let $\mathcal{S}$ be an* ***autonomous*** *Hamiltonian system and consider the motion of the phase points that initially lie in a bounded region $\mathcal{R}_0$ of the phase space. If the paths of all of these points lie within a fixed* ***bounded*** *region of phase space for all time, then some of the points must eventually return to $\mathcal{R}_0$.*

Proof. Let $\mathcal{R}_1$ be the region occupied by the points after time τ. (We will suppose that $\mathcal{R}_1$ does not overlap $\mathcal{R}_0$ so that all the points that lay in $\mathcal{R}_0$ at time $t = 0$ have left $\mathcal{R}_0$ at time $t = \tau$.) We must show that some of them eventually return to $\mathcal{R}_0$. Let $\mathcal{R}_2, \mathcal{R}_3, \ldots, \mathcal{R}_n$ be the regions occupied by the same points after times $2\tau, 3\tau, \ldots, n\tau$. By Liouville's theorem, *all of these regions have the same volume*. Therefore, if they never overlap, their total volume will increase without limit. But, by assumption, all these regions lie within some *finite* volume, so that eventually one of them must overlap a previous one. This much is obvious, but we must now show that an overlap takes place with the *original* region $\mathcal{R}_0$.

Suppose it is $\mathcal{R}_m$ that overlaps $\mathcal{R}_k$ $(0 \leq k < m)$. Each point of this overlap region corresponds to an intersection of the paths of two phase points that started out at some points $\boldsymbol{x}_1$, $\boldsymbol{x}_2$ of $\mathcal{R}_0$ at time $t = 0$. In the same notation used in the proof of Liouville's theorem, it means that $\boldsymbol{X}(\boldsymbol{x}_1, m\tau) = \boldsymbol{X}(\boldsymbol{x}_2, k\tau)$. But, since the system is **autonomous**, the two solutions $\boldsymbol{X}(\boldsymbol{x}_1, t)$ and $\boldsymbol{X}(\boldsymbol{x}_2, t)$ must therefore differ only by a shift $(m - k)\tau$ in the origin of time. It follows that $\boldsymbol{X}(\boldsymbol{x}_1, (m - k)\tau) = \boldsymbol{X}(\boldsymbol{x}_2, 0) = \boldsymbol{x}_2$. Thus the phase point that was at $\boldsymbol{x}_1$ when $t = 0$ is at $\boldsymbol{x}_2$ when $t = (m - k)\tau$. This phase point has therefore returned to $\mathcal{R}_0$ after time $(m - k)\tau$ and this completes the proof. ■

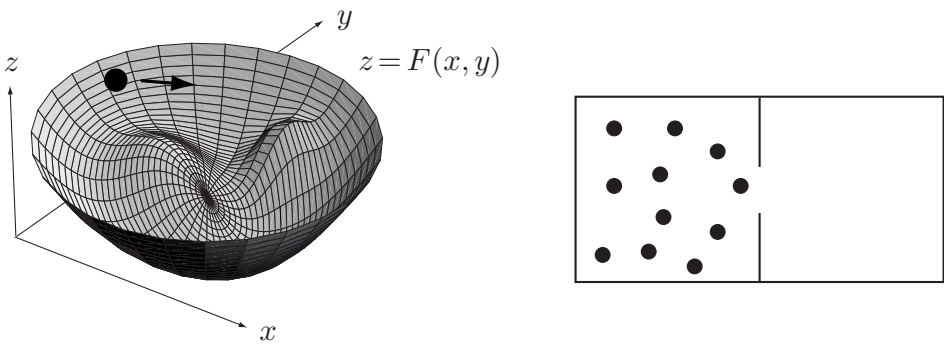

FIGURE 14.4 Consequences of Poincaré's recurrence theorem. **Left**: the particle sliding inside the smooth irregular bowl will eventually almost reassume its initial state. **Right**: The mole of gas molecules, initially all in the left compartment will eventually all be found there again.

Since the recurrence theorem holds for any sub-region of $\mathcal{R}_0$, it follows that, throughout $\mathcal{R}_0$, there are phase points that pass *arbitrarily close* to their original positions. Thus if the system $\mathcal{S}$ has one of these points as its initial state, then $\mathcal{S}$ will eventually become arbitrarily close to reassuming that state. Actually, such points are typical rather than exceptional. To show this requires a stronger version of Poincaré's theorem* than we have proved here, namely: *The path of* ***almost every***† *point in* $\mathcal{R}_0$ *passes* ***arbitrarily close*** *to its starting point*. This implies the remarkable result that *for amost every choice of the initial conditions, the system* $\mathcal{S}$ *becomes arbitrarily close to reassuming those conditions at later times*.

An example of this phenomenon is the motion of a single particle P sliding under gravity on the smooth inner surface of a bowl of some irregular shape $z = F(x, y)$, as shown in Figure 14.4. This is an autonomous Hamiltonian system with two degrees of freedom. Take the Cartesian coordinates (x, y) of P to be generalised coordinates. Then the Lagrangian is given by

$$\begin{aligned} L &= \tfrac{1}{2}m\left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right) - mgz \\ &= \tfrac{1}{2}m\left(\dot{x}^2 + \dot{y}^2 + (F_{,x}\,\dot{x} + F_{,y}\,\dot{y})^2\right) - mgF, \end{aligned}$$

where $F_{,x} = \partial F/\partial x$ and $F_{,y} = \partial F/\partial y$. The conjugate momenta are

$$p_x = m\left(\dot{x} + (F_{,x}\,\dot{x} + F_{,y}\,\dot{y})F_{,x}\right), \qquad p_y = m\left(\dot{y} + (F_{,x}\,\dot{x} + F_{,y}\,\dot{y})F_{,y}\right).$$

Just because energy is conserved, it does not necessarily mean that Poincaré's theorem applies. We must show that the energy surfaces in phase space are bounded. The proof of this is as follows:

* See Walters [12].

† This means that the set of exceptional points has measure zero. For example, in a two-dimensional phase space, a curve has zero measure.

In this case, $\mathcal{R}_0$ is some bounded region of the phase space (x, y, p_x, p_y). Suppose that z_0 is the maximum value of z and that T_0 is the maximum kinetic energy associated with points of $\mathcal{R}_0$. Then, by energy conservation, the maximum value of z in the subsequent motions cannot exceed $z^{\max} = z_0 + (T_0/mg)$. Hence, providing the bowl rises to at least this height, the motions are confined to values of (x, y) that satisfy $F(x, y) \leq z^{\max}$. It follows that both x and y are bounded in the subsequent motions. Also, if the lowest point of the bowl is at $z = 0$, the value of T in the subsequent motions cannot exceed $T^{\max} = T_0 + mgz_0$. It follows that $\dot{x}$ and $\dot{y}$ are bounded in the subsequent motions and this implies that the same is true for p_x and p_y. Hence x, y, p_x, and p_y are all bounded in the subsequent motions. This means that that the paths of the phase points that lie in $\mathcal{R}_0$ when $t = 0$ are confined to a bounded region of the phase space for all time. **Poincaré's theorem therefore applies**.

Hence, if the particle P is released from rest (say) at some point A on the surface of the bowl, then, whatever the shape of the bowl, P will become arbitrarily close to being at rest at A at later times.

In the same way, it follows that if a compartment containing a mole of gas molecules is separated from an empty compartment by a partition, and the partition is suddenly punctured, then at (infinitely many!) later times the molecules will *all be found in the first compartment again*. This remarkable result, which seems to be in contradiction to the second law of thermodynamics, appears less paradoxical when one realises that 'later times' may mean 10^{20} years later!

Question ***Exceptional points***

How do you know that the initial conditions you have chosen do not correspond to an 'exceptional point' for which Poincaré's theorem does not hold?

Answer

You don't know, but you would be very unlucky if this happened! ■

Problems on Chapter 14

Answers and comments are at the end of the book.

Harder problems carry a star (∗).

Finding Hamiltonians

14.1 Find the Legendre transform $G(v_1, v_2, w)$ of the function

$$F(u_1, u_2, w) = 2u_1^2 - 3u_1u_2 + u_2^2 + 3wu_1,$$

where w is a passive variable. Verify that $\partial F/\partial w = -\partial G/\partial w$.

14.2 A smooth wire has the form of the helix $x = a\cos\theta$, $y = a\sin\theta$, $z = b\theta$, where θ is a real parameter, and a, b are positive constants. The wire is fixed with the axis Oz pointing vertically upwards. A particle P of mass m can slide freely on the wire. Taking θ as generalised coordinate, find the Hamiltonian and obtain Hamilton's equations for this system.

14.3 ***Projectile*** Using Cartesian coordinates, find the Hamiltonian for a projectile of mass m moving under uniform gravity. Obtain Hamilton's equations and identify any cyclic coordinates.

14.4 ***Spherical pendulum*** The spherical pendulum is a particle of mass m attached to a fixed point by a light inextensible string of length a and moving under uniform gravity. It differs from the simple pendulum in that the motion is not restricted to lie in a vertical plane. Show that the Lagrangian is

$$L = \tfrac{1}{2}ma^2\left(\dot{\theta}^2 + \sin^2\theta\,\dot{\phi}^2\right) + mga\cos\theta,$$

where the polar angles θ, ϕ are shown in Figure 11.7. Find the Hamiltonian and obtain Hamilton's equations. Identify any cyclic coordinates.

14.5 The system shown in Figure 10.9 consists of two particles P_1 and P_2 connected by a light inextensible string of length a. The particle P_1 is constrained to move along a fixed smooth horizontal rail, and the whole system moves under uniform gravity in the vertical plane through the rail. For the case in which the particles are of equal mass m, show that the Lagrangian is

$$L = \tfrac{1}{2}m\left(2\dot{x}^2 + 2a\dot{x}\dot{\theta} + a^2\dot{\theta}^2\right) + mga\cos\theta,$$

where x and θ are the coordinates shown in Figure 10.9.

Find the Hamiltonian and verify that it satisfies the equations $\dot{x} = \partial H/\partial p_x$ and $\dot{\theta} = \partial H/\partial p_\theta$. [Messy algebra.]

14.6 ***Pendulum with a shortening string*** A particle is suspended from a support by a light inextensible string which passes through a small fixed ring vertically below the support. The particle moves in a vertical plane with the string taut. At the same time, the support is made to move vertically having an upward displacement $Z(t)$ at time t. The effect is that the particle oscillates like a simple pendulum whose string length at time t is $a - Z(t)$, where a is a positive constant. Show that the Lagrangian is

$$L = \tfrac{1}{2}m\left((a - Z)^2\dot{\theta}^2 + \dot{Z}^2\right) + mg(a - Z)\cos\theta,$$

where θ is the angle between the string and the downward vertical.

Find the Hamiltonian and obtain Hamilton's equations. Is H conserved?

14.7 ***Charged particle in an electrodynamic field*** The Lagrangian for a particle with mass m and charge e moving in the general electrodynamic field $\{\boldsymbol{E}(\boldsymbol{r}, t), \boldsymbol{B}(\boldsymbol{r}, t)\}$ is given in Cartesian coordinates by

$$L(\boldsymbol{r}, \dot{\boldsymbol{r}}, t) = \tfrac{1}{2}m\,\dot{\boldsymbol{r}}\cdot\dot{\boldsymbol{r}} - e\,\phi(\boldsymbol{r}, t) + e\,\dot{\boldsymbol{r}}\cdot\boldsymbol{A}(\boldsymbol{r}, t),$$

where $\boldsymbol{r} = (x, y, z)$ and $\{\phi, \boldsymbol{A}\}$ are the electrodynamic potentials of field $\{\boldsymbol{E}, \boldsymbol{B}\}$. Show that the corresponding Hamiltonian is given by

$$H(\boldsymbol{r}, \boldsymbol{p}, t) = \frac{(\boldsymbol{p} - e\boldsymbol{A})\cdot(\boldsymbol{p} - e\boldsymbol{A})}{2m} + e\,\phi,$$

where $\boldsymbol{p} = (p_x, p_y, p_x)$ are the generalised momenta conjugate to the coordinates (x, y, z). [Note that $\boldsymbol{p}$ is *not* the ordinary linear momentum of the particle.] Under what circumstances is H conserved?

14.8 ***Relativistic Hamiltonian*** The relativistic Lagrangian for a particle of rest mass m_0 moving along the x-axis under the potential field $V(x)$ is given by

$$L = m_0 c^2 \left(1 - \left(1 - \frac{\dot{x}^2}{c^2}\right)^{1/2}\right) - V(x).$$

Show that the corresponding Hamiltonian is given by

$$H = m_0 c^2 \left(1 + \left(\frac{p_x}{m_0 c}\right)^2\right)^{1/2} - m_0 c^2 + V(x),$$

where p_x is the generalised momentum conjugate to x.

14.9 ***A variational principle for Hamilton's equations*** Consider the functional

$$J[\boldsymbol{q}(t), \boldsymbol{p}(t)] = \int_{t_0}^{t_1} \Big(H(\boldsymbol{q}, \boldsymbol{p}, t) + \boldsymbol{q} \cdot \dot{\boldsymbol{p}} - \dot{\boldsymbol{q}} \cdot \boldsymbol{p}\Big)\, dt$$

of the $2n$ independent functions $q_1(t), \ldots, q_n(t),\ p_1(t), \ldots, p_n(t)$. Show that the extremals of J satisfy Hamilton's equations with Hamiltonian H.

Liouville's theorem and recurrence

14.10 In the theory of dynamical systems, a point is said to be an *asymptotically stable equilibrium point* if it 'attracts' points in a nearby volume of the phase space. Show that such points cannot occur in Hamiltonian dynamics.

14.11 A one dimensional damped oscillator with coordinate q satisfies the equation $\ddot{q} + 4\dot{q} + 3q = 0$, which is equivalent to the first order system

$$\dot{q} = v, \qquad \dot{v} = -3q - 4v.$$

Show that the area $a(t)$ of any region of points moving in (q, v)-space has the time variation

$$a(t) = a(0)\, e^{-4t}.$$

Does this result contradict Liouville's theorem?

14.12 ***Ensembles in statistical mechanics*** In statistical mechanics, a macroscopic property of a system $\mathcal{S}$ is calculated by averaging that property over a set, or *ensemble*, of points moving in the phase space of $\mathcal{S}$. The number of ensemble points in any volume of phase space is represented by a *density function* $\rho(\boldsymbol{q}, \boldsymbol{p}, t)$. If the system is autonomous and in *statistical equilibrium*, it is required that, even though the ensemble points are moving (in accordance with

Hamilton's equations), their density function should remain the same, that is, $\rho = \rho(\boldsymbol{q}, \boldsymbol{p})$. This places a restriction on possible choices for $\rho(\boldsymbol{q}, \boldsymbol{p})$. Let $\mathcal{R}_0$ be any region of the phase space and suppose that, after time t, the points of $\mathcal{R}_0$ occupy the region $\mathcal{R}_t$. Explain why statistical equilibrium requires that

$$\int_{\mathcal{R}_0} \rho(\boldsymbol{q}, \boldsymbol{p})\, dv = \int_{\mathcal{R}_t} \rho(\boldsymbol{q}, \boldsymbol{p})\, dv$$

and show that the *uniform* density function $\rho(\boldsymbol{q}, \boldsymbol{p}) = \rho_0$ satisfies this condition. [It can be proved that the above condition is also satisfied by any density function that is constant along the streamlines of the phase flow.]

14.13 Decide if the energy surfaces in phase space are bounded in the following cases:

(i) The two-body gravitation problem with $E < 0$.

(ii) The two-body gravitation problem viewed from the zero momentum frame and with $E < 0$.

(iii) The three-body gravitation problem viewed from the zero momentum frame and with $E < 0$. Does the solar system have the recurrence property?

Poisson brackets

14.14 ***Poisson brackets*** Suppose that $u(\boldsymbol{q}, \boldsymbol{p})$ and $v(\boldsymbol{q}, \boldsymbol{p})$ are any two functions of position in the phase space $(\boldsymbol{q}, \boldsymbol{p})$ of a mechanical system $\mathcal{S}$. Then the **Poisson bracket** $[u, v]$ of u and v is defined by

$$[u, v] = \operatorname{grad}_{\boldsymbol{q}} u \cdot \operatorname{grad}_{\boldsymbol{p}} v - \operatorname{grad}_{\boldsymbol{p}} u \cdot \operatorname{grad}_{\boldsymbol{q}} v = \sum_{j=1}^{n} \left(\frac{\partial u}{\partial q_j} \frac{\partial v}{\partial p_j} - \frac{\partial u}{\partial p_j} \frac{\partial v}{\partial q_j} \right).$$

The *algebraic* behaviour of the Poisson bracket of two functions resembles that of the cross product $\boldsymbol{U} \times \boldsymbol{V}$ of two vectors or the commutator $\boldsymbol{UV} - \boldsymbol{VU}$ of two matrices. The Poisson bracket of two functions is closely related to the commutator of the corresponding operators in quantum mechanics.*

Prove the following properties of Poisson brackets.

Algebraic properties

$$[u, u] = 0, \qquad [v, u] = -[u, v], \qquad [\lambda_1 u_1 + \lambda_2 u_2, v] = \lambda_1 [u_1, v] + \lambda_2 [u_2, v]$$

$$[[u, v], w] + [[w, u], v] + [[v, w], u] = 0.$$

This last formula is called *Jacobi's identity*. It is quite important, but there seems to be no way of proving it apart from crashing it out, which is very tedious. Unless you can invent a smart method, leave this one alone.

* The commutator $[\mathbf{U}, \mathbf{V}]$ of two quantum mechanical operators $\mathbf{U}, \mathbf{V}$ corresponds to $i\hbar[u, v]$, where $\hbar$ is the modified Planck constant, and $[u, v]$ is the Poisson bracket of the corresponding classical variables u, v.

Fundamental Poisson brackets

$$[q_j, q_k] = 0, \qquad [p_j, p_k] = 0, \qquad [q_j, p_k] = \delta_{jk},$$

where δ_{jk} is the Kroneker delta.

Hamilton's equations

Show that Hamilton's equations for $\mathcal{S}$ can be written in the form

$$\dot{q}_j = [q_j, H], \qquad \dot{p}_j = [p_j, H], \qquad (1 \leq j \leq n).$$

Constants of the motion

(i) Show that the *total* time derivative of $u(\boldsymbol{q}, \boldsymbol{p})$ is given by

$$\frac{du}{dt} = [u, H]$$

and deduce that u is a constant of the motion of $\mathcal{S}$ if, and only if, $[u, H] = 0$.

(ii) If u and v are constants of the motion of $\mathcal{S}$, show that the Poisson bracket $[u, v]$ is another constant of the motion. [Use Jacobi's identity.] Does this mean that you can keep on finding more and more constants of the motion ?

14.15 ***Integrable systems and chaos*** A mechanical system is said to be **integrable** if its equations of motion are soluble in the sense that they can be reduced to integrations. (You do not need to be able to evaluate the integrals in terms of standard functions.) A theorem due to Liouville states that *any Hamiltonian system with n degrees of freedom is integrable if it has n independent constants of the motion, and all these quantities commute in the sense that all their mutual Poisson brackets are zero*.* The qualitative behaviour of integrable Hamiltonian systems is well investigated (see Goldstein [4]). In particular, *no integrable Hamiltonian system can exhibit chaos*.

Use Liouville's theorem to show that any autonomous system with n degrees of freedom and $n - 1$ cyclic coordinates must be integrable.

Computer assisted problem

14.16 ***The three body problem***

There is no general solution to the problem of determining the motion of three or more bodies moving under their mutual gravitation. Here we consider a restricted case of the three-body problem in which the mass of one of the bodies, P, is *much smaller* than that of the other two masses, which are called the primaries. In this case we neglect the effect of P on the primaries which therefore move in known fixed orbits. The body P moves in the time dependent, gravitational field of the primaries.

* This result is really very surprising. A *general* system of first order ODEs in $2n$ variables needs $2n$ integrals in order to be integrable in the Liouville sense. Hamiltonian systems need only half that number. The theorem does not rule out the possibility that that there could be other classes of integrable systems. However, according to Arnold [2], every system that has ever been integrated is of the Liouville kind!

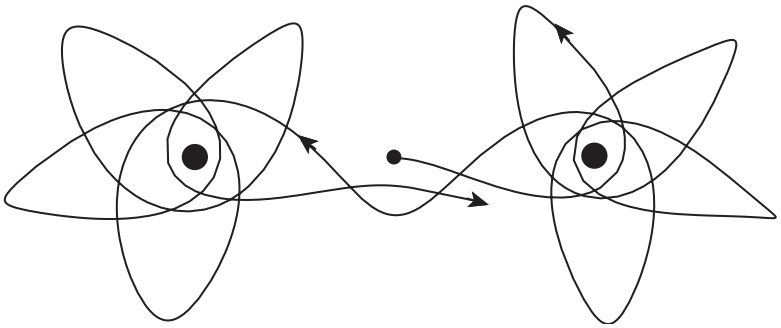

FIGURE 14.5 There is no such thing as a typical orbit in the three-body problem. The orbit shown corresponds to the initial conditions $x = 0$, $y = 0$, $p_x = 1.03$, $p_y = 0$ and is viewed from axes *rotating with the primaries*.

Suppose the primaries each have mass M and move under their mutual gravitation around a fixed circle of radius a, being at the opposite ends of a rotating diameter. The body P moves under the gravitational attraction of the primaries in the same plane as their circular orbit. Using Cartesian coordinates, write code to set up Hamilton's equations for this system and solve them with general initial conditions. [Take M as the unit of mass, a as the unit of length, and take the unit of time so that the speed of the primaries is unity. With this choice of units, the gravitational constant $G = 4$.]

By experimenting with different initial conditions, some very weird orbits can be found for P. It is interesting to plot these relative to fixed axes and also relative to axes rotating with the primaries, as in Figure 14.5. Some fascinating cases are shown by Acheson [] and you should be able to reproduce these. [Acheson used a different normalisation however and his initial data needs to be doubled to be used in your code.]